

TOPICAL REVIEW

 $W = 0$ pairing in Hubbard and related models of low-dimensional superconductorsAdalberto Balzarotti ^{*}, Michele Cini ^{*††} and Enrico Perfetto ^{*†}, and Gianluca Stefanucci[‡]^{*} Istituto Nazionale per la Fisica della Materia, Dipartimento di Fisica, Università di Roma Tor Vergata, via della ricerca Scientifica 1, 00133 Roma Italy[†] INFN - Laboratori Nazionali di Frascati, Via E. Fermi 40, 00044 Frascati, Italy[‡] Department of Solid State Theory, Institute of Physics, Lund University, Sölvegatan 14 A, 22362 Lund Sweden

Abstract. Lattice Hamiltonians with on-site interaction W have $W = 0$ solutions, that is, many-body *singlet* eigenstates without double occupation. In particular, $W = 0$ pairs give a clue to understand the pairing force in repulsive Hubbard models. These eigenstates are found in systems with high enough symmetry, like the square, hexagonal or triangular lattices. By a general theorem, we propose a systematic way to construct all the $W = 0$ pairs of a given Hamiltonian. We also introduce a canonical transformation to calculate the effective interaction between the particles of such pairs. In geometries appropriate for the CuO_2 planes of cuprate superconductors, armchair Carbon nanotubes or Cobalt Oxides planes, the dressed pair becomes a bound state in a physically relevant range of parameters. We also show that $W = 0$ pairs quantize the magnetic flux like superconducting pairs do. The pairing mechanism breaks down in the presence of strong distortions. The $W = 0$ pairs are also the building blocks for the antiferromagnetic ground state of the half-filled Hubbard model at weak coupling. Our analytical results for the 4×4 Hubbard square lattice, compared to available numerical data, demonstrate that the method, besides providing intuitive grasp on pairing, also has quantitative predictive power. We also consider including phonon effects in this scenario. Preliminary calculations with small clusters indicate that vector phonons hinder pairing while half-breathing modes are synergic with the $W = 0$ pairing mechanism both at weak coupling and in the polaronic regime.

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1. Introduction

In the last decades, much effort has been devoted to *exotic* mechanisms of pairing and to the possibility of non-conventional superconductivity in new materials. In a list of the most important and frequently discussed examples, one could mention the cuprates[1], organic superconductors including fullerenes[2] and carbon nanotubes[3], ruthenates[4], and Na-Co oxides[5]. Among the most interesting possibilities, correlation effects have been invoked, and the Hubbard model[6] has been increasingly popular to achieve a simplified picture.

The Hubbard model is believed to exhibit various interesting phenomena including antiferromagnetism, ferrimagnetism, ferromagnetism, metal-insulator transitions, etc. It is the simplest Hamiltonian covering both aspects of a strongly correlated electron system (like the CuO_2 planes of cuprates), namely the competition between band-like behaviour and the tendency to atomic-like localisation driven by the screened Coulomb repulsion. Besides, several authors believe that it can exhibit a superconducting phase

in a certain parameters regime. Despite its simplicity, the Hubbard Hamiltonian cannot be exactly solved in more than 1d and a large variety of approaches has been proposed to study the superconducting correlations in the ground state and at finite temperature. Bickers and co-workers[7] were among the first to propose the $d_{x^2-y^2}$ wave superconductivity in 2d. A recent survey of the superconducting properties of the single- and multi-band Hubbard model can be found in Ref.[8].

Another popular class of models are that obtained from the Hubbard Hamiltonian in the strong coupling limit. A large on-site Coulomb repulsive energy U between carriers of opposite spins tends to reduce the double occupancy. A straightforward perturbation theory in the parameters t of the kinetic term leads to Heisenberg-like Hamiltonians for fermions propagating through an antiferromagnetic background with an exchange interaction J between neighbouring spins. These are the so called t-J models[9],[10]. In the t-J model the double-occupancy is forbidden by the so called Gutzwiller projection[11], and there is no on-site repulsion. However, superconductivity is a delicate phenomenon and the exclusion of double occupied sites costs kinetic energy, so the t-J model might fail to give an appropriate description of the Hubbard model when U is comparable to t .

In this review article, we illustrate the “ $W = 0$ ” pairing mechanism, in which symmetry is capable of cutting down the on-site repulsion from the outset, without any need of the Gutzwiller projection. This effect works at any U/t and it relies on a configuration mixing which entails the presence of degenerate one-body states at the Fermi level. Moreover, we provide evidence that this configuration mixing, when applied to the full many-body problem, can produce pairing when physical parameter values are used.

The pairing force in the Hubbard model is induced by repulsive interactions, and recalls the Kohn-Luttinger[12] pairing in the Jellium. They pointed out that any three-dimensional Fermi liquid undergoes a superconducting instability by Cooper pairs of parallel spins and very large relative angular momentum l . A simplified view of the Kohn-Luttinger effect is given by considering one particle of the pair as an external charge. Then, the screening gives rise to a long-range oscillatory potential (Friedel oscillations) due to the singularity of the longitudinal dielectric function at $2k_F$; here k_F is the Fermi wavevector. The strict reasoning exploits the fact that the Legendre expansion coefficients of any regular direct interaction between particles of opposite momentum drops off exponentially in l . On the other hand, the second-order contribution to the scattering amplitude falls as $1/l^4$ and at least for odd l leads to an attractive interaction. In the modern renormalization group language[13], the second-order correction is obtained by summing up the marginal scattering amplitudes of the isotropic Fermi liquid coming from the so-called Forward channels, including, for antiparallel spins, a spin-flip diagram. This scenario does not work in the two-dimensional Fermi liquid, but going beyond the second-order perturbation theory the Kohn-Luttinger effect is recovered[14].

The present mechanism works with singlet pairs and differs from Kohn-Luttinger

one in other important ways. In contrast with the homogeneous electron gas, the lattice structure gives very tight pairs and the $W = 0$ mechanism displays very clearly in tiny clusters as well. On top of that, it is worth noticing that in high- T_C superconductors the size of the Cooper pairs is expected to be of the order of few lattice constants and hence the pairing mechanism should lend itself to cluster studies. Macroscopically large lattices with periodic boundary conditions have large symmetry groups including the space groups (point symmetry + translational symmetry); in such conditions, the $W = 0$ pairing mechanism is at its best. Similarly, in finite geometries, the largest binding energy is obtained in fully symmetric clusters while static distortions tend to unbind the pair. Exact calculations on finite models should bring to light interesting aspects of the microscopic origin of the pairing mechanism, and be useful as tests for the analytic developments.

To test the superconducting nature of the pairs arising from repulsive interactions, one can use finite systems in *gedanken* experiments. We probe the behaviour of $W = 0$ pairs in the presence of a static magnetic field and we show that they produce diamagnetic supercurrents that screen the vector potential. As a result the superconducting flux quantization is observed in various geometries.

The paper is organised as follows. In Section 2, we review the pairing mechanism in small symmetric clusters. We prove the existence of two-body singlet eigenstates with vanishing on-site Hubbard repulsion, that we call $W = 0$ pairs. We have collected in Subsection 2.2 the somewhat more technical aspects, which are central for the mathematical foundation of the theory, while readers who are only interested in the phenomenology might skip it. We prove a general theorem on the allowed symmetries of such pairs. From the theorem we extract a practical recipe to build $W = 0$ pairs in any symmetric geometry (finite or macroscopically large). A careful analysis on the smallest “allowed” cluster, the CuO_4 , shows that pairing can be obtained in a physical parameter range. The underlying pairing mechanism is investigated using many-body perturbation theory. In Section 3 we generalise the theory to arbitrary large systems. We introduce a non-perturbative canonical transformation leading to an effective Hamiltonian for the pair. The method is free from the limitations of perturbation theory; the relation of the present formalism to Cooper theory from one side and to cluster results from the other is discussed. Two kinds of bound states of different symmetries result, and the dependence of the binding energy on the filling and other parameters is explored. In Section 4 we study the Hubbard Model at half filling. We remove the ground-state degeneracy in first order perturbation theory by means of a suitable *local* formalism. We show that the ground state is the spin singlet projection of a determinantal state exhibiting the *antiferromagnetic property*: the translation by a lattice step is equivalent to a spin flip. As an illustration, the 4×4 square lattice is studied in detail. The half filled antiferromagnetic ground state is doped with two holes and an effective interaction between them is derived by means of the canonical transformation. The analytical results agree well with the numerical ones and this shows the predictive power of the approach. In Section 5 we investigate the $W = 0$ pairing mechanism in carbon nanotubes

and triangular cobalt oxides. Section 6 is aimed to study the superconducting magnetic response of symmetric Hubbard models with $W = 0$ bound pairs. Section 7 deals with the inclusion of the lattice degrees of freedom; we show that phonons give a synergic contribution to the purely electronic mechanism and catastrophic Jahn-Teller distortions do not occur. Finally, we draw our conclusions and outlook in Section 8.

2. Pairing in the Hubbard Model

In this review, we shall deal with Hubbard-like models of various geometries, designed for application to superconducting strongly correlated materials. The prototype Hubbard Hamiltonian reads

$$H = K + W = t \sum_{\langle i,j \rangle, \sigma} c_{j\sigma}^\dagger c_{i\sigma} + U \sum_i n_{i\uparrow} n_{i\downarrow}, \quad (1)$$

where K stands for the kinetic energy while W accounts for the on-site repulsive interaction. The summation on $\langle i, j \rangle$ runs over sites i and j which are nearest neighbours.

In Eq. (1) the interaction term is repulsive and there is no electron-phonon coupling, so the very existence of pairing is a paradox. An effective attractive force comes from, e.g., the exchange of spin fluctuations but it must be stronger than the direct Hubbard repulsion to give rise a bound pair. Bickers and co-workers[7] explored the consequences of a spin density wave instability on such a pairing force within the RPA approximation. They found a superconducting phase with pair-wavefunctions of $d_{x^2-y^2}$ symmetry in the 2d Hubbard model. The next level of calculations were carried out by using the FLEX approximation[15]. This method treats the fluctuations in the magnetic, density and pairing channels in a self-consistent and conserving way. It was found that the antiferromagnetic fluctuations lead to a superconducting phase of $d_{x^2-y^2}$ symmetry which neighbours the SDW phase, in accordance with the previous findings.

The phase diagram becomes less clear close to half filling because of the numerous infrared divergencies due to the nesting of the Fermi surface and Van Hove singularities. As a consequence, the results of any many-body treatment depend on the choice of diagrams to be summed. Renormalization Group (RG) methods[13] are a well controlled alternative approach to deal with Fermi systems having competing singularities. The RG has been used by several authors[16],[17],[18] to study the coupling flows at different particle densities. In agreement with the previous findings, RG calculations show a d -wave superconducting instability away from half filling. The underlying physical mechanism, namely exchange of spin- or charge-density fluctuations, is also the same as in the FLEX approach.

Despite such evidence, there is no general agreement on the existence of a superconducting phase in the Hubbard model[19],[20],[21]. In order to clarify such a controversy it is very useful to have exact data to rely on. Unfortunately, the one band Hubbard model is exactly solved only in one spatial dimension[22] and no sign of superconductivity was found there[23]. Very few exact analytical results are available for the 2 dimensional case[24]. Therefore in 2 dimensions the low-lying states must be

explored by means of exact diagonalizations on finite clusters. This kind of numerical calculation, complemented by analytical work and physical insight, may bring to light interesting local aspects of the microscopic pairing mechanism.

The exact ground state of several small Hubbard systems have been numerically found by means of Lanczos and quantum Monte Carlo techniques. A pairing criterion that we shall discuss below was given by Richardson in the context of nuclear physics[29]. Defining

$$\tilde{\Delta}(N+2) = E(N+2) + E(N) - 2E(N+1) \quad (2)$$

where $E(N)$ is the N -body ground state energy,

$$\tilde{\Delta}(N+2) < 0 \quad (3)$$

signals a bound pair in the ground state with $N+2$ particles and $|\tilde{\Delta}|$ is interpreted as the binding energy of the pair. Pairing was found under various conditions by several authors[30],[31], and among the geometries considered the 4×4 system[32] is one of the most relevant for studying the pairing instability close to the antiferromagnetic phase.

Below, we derive an analytic theory of pairing interactions, and report several detailed case studies where the formulas are validated by comparison with the numerical data. The results support general qualitative criteria for pairing induced by the on-site repulsion only. This shows that our approach successfully predicts the formation of bound pairs, and explains why other ingredients like strong off-site interactions are needed in other geometries. The analytic approach is also needed to predict what happens for large systems and in the thermodynamic limit. Increasing the cluster size the computed pair binding energies show a rapid decrease, and several authors on the basis of the numerical data consider pairing in the Hubbard model as a size effect. Unfortunately, the number of configurations grows in a prohibitive way with the cluster size[33] and numerical data currently available on 4×4 or even 6×6 clusters cannot provide reliable extrapolations to the bulk limit. In Section 3.4 we show that we understand the trend analytically very well, that much larger cells (at least 30×30) are needed to estimate the asymptotic behaviour and that we have reasons to believe that pairing with a reduced but substantial binding energy persists in the full plane.

2.1. $W = 0$ Pairing in Cu-O Clusters

In this Section, we illustrate the concept of $W = 0$ pairs and the way they become bound states, by using examples with a geometry relevant for the cuprates. Our starting point is the three-band Hubbard Hamiltonian

$$H = K + W + W_{\text{off-site}} \quad (4)$$

where

$$K = t \sum_{\langle ij \rangle, \sigma} (p_{j\sigma}^\dagger d_{i\sigma} + \text{h.c.}) + t_{pp} \sum_{\langle jj' \rangle, \sigma} p_{j\sigma}^\dagger p_{j'\sigma} + \varepsilon_d \sum_{i, \sigma} n_{i\sigma} + \varepsilon_p \sum_{j, \sigma} n_{j\sigma}$$

C_{4v}	1	C_2	$C_4^{(+)}, C_4^{(-)}$	σ_x, σ_y	σ_+, σ_-	Symmetry
A_1	1	1	1	1	1	$x^2 + y^2$
A_2	1	1	1	-1	-1	$(x/y) - (y/x)$
B_1	1	1	-1	1	-1	$x^2 - y^2$
B_2	1	1	-1	-1	1	xy
E	2	-2	0	0	0	(x, y)

Table 1. Character table of the C_{4v} symmetry Group. Here **1** denotes the identity, C_2 the 180 degrees rotation, $C_4^{(+)}, C_4^{(-)}$ the counterclockwise and clockwise 90 degrees rotation, σ_x, σ_y the reflection with respect to the $y = 0$ and $x = 0$ axis and σ_+, σ_- the reflection with respect to the $x = y$ and $x = -y$ diagonals. The C_{4v} symmetry Group has 4 one-dimensional irreducible representations (irreps) A_1, A_2, B_1, B_2 and 1 two-dimensional irrep E . In the last column it is shown how each of them transforms under C_{4v} .

and

$$W = U_d \sum_i n_{i\uparrow} n_{i\downarrow} + U_p \sum_j n_{j\uparrow} n_{j\downarrow}, \quad W_{\text{off-site}} = U_{pd} \sum_{\langle ij \rangle, \sigma\sigma'} n_{i\sigma} n_{j\sigma'}.$$

Here, p_j (d_i) are fermionic operators that destroy holes at the Oxygen (Copper) ions labelled j (i) and $n = p^\dagger p$ ($= d^\dagger d$) is the number operator. $\langle ij \rangle$ refers to pairs of nearest neighbors i (Copper) and j (Oxygen) sites. The hopping terms correspond to the hybridization between nearest neighbors Cu and O atoms, and are roughly proportional to the overlap between localized Wannier orbitals.

The parameters U_d and U_p are positive constants that represent the repulsion between holes when they are at the same Copper (d) and Oxygen (p) orbitals, respectively. U_{pd} has a similar meaning, *i.e.*, it corresponds to the Coulombic repulsion when two holes occupy two adjacent Cu-O sites. The on-site energies ε_p and ε_d refer to the occupied orbitals of Oxygen and Copper. In the strong coupling limit, and with one particle per unit cell, this model reduces to the spin Heisenberg Model with a superexchange antiferromagnetic coupling[39],[40].

From a band structure calculation and by best fitting the results of *ab initio* calculations[41] one can roughly estimate the actual values of the parameters in the Hamiltonian of Eq. (4). Our preferred set is (in eV): $\varepsilon_p - \varepsilon_d = 3.5$, $t = 1.3$, $t_{pp} = -0.65$, $U_d = 5.3$, $U_p = 6$ and, most probably, $U_{pd} < 1.2$.

As Cini and Balzarotti[34] pointed out, highly symmetric clusters possess 2-holes singlet eigenstates of H which do not feel the on-site repulsion W ; such eigenstates were called $W = 0$ *pairs* and play a crucial role for pairing. In order to have $W = 0$ solutions, the clusters must possess the full C_{4v} (square) symmetry, and must be centered around a Cu site. Group arguments are central to our approach and we show the Characters of the C_{4v} Group in Table 1. The symmetry requirements are so stringent that clusters with such properties had not been studied previously. In particular, the present discussion does not apply to the geometries, like those examined by Hirsch *et al.*[35],[36] and Balseiro *et al.*[30], which are *forbidden* from our viewpoint. The Cu_4O_4

ε_{A_1}	ε_{E_x}	ε_{E_y}	ε_{B_1}	$\varepsilon_{A'_1}$
$\tau - \sqrt{4 + \tau^2}$	0	0	-2τ	$\tau + \sqrt{4 + \tau^2}$

Table 2. One-body levels of the CuO_4 cluster in units of t as a function of the dimensionless parameter $\tau \equiv t_{pp}/t$.

geometry considered by Ogata and Shiba[37] has the C_{4v} symmetry, but lacks the central Cu, and therefore it is *forbidden*. Those built from degenerate one-body levels are not $W = 0$ pairs; they feel the on-site repulsion U_p on the Oxygen sites, and yield $\tilde{\Delta} < 0$ only if U_p is very small[34],[38].

Note that we are using the same t for all Cu-O bonds, while some authors use other conventions. For instance, F. C. Zhang and T. M. Rice[42] use an alternating sign prescription for t , which may be obtained by changing the sign of all the O orbitals in the horizontal lines containing Cu ions. The two pictures are related by a gauge transformation, under which the orbital symmetry labels A_1 and B_1 are interchanged. Some of the symmetry related information is gauge dependent and unobservable, while some is physical (e.g. degeneracies are).

The reason why symmetry is so basic for our mechanism is that the $W = 0$ two-body eigenstates arise when two holes occupy degenerate one-body levels. When such degenerate states are partially filled in the many-body ground state, bound pairs can form. The *interacting ground state* must be described in terms of a many-body configuration mixing, but the presence of the $W = 0$ pair imparts to the many-body state a special character; it can be described in terms of a bound pair moving on a closed-shell background. This is the main point that we want to make, and it is deeply related to the symmetry quantum numbers.

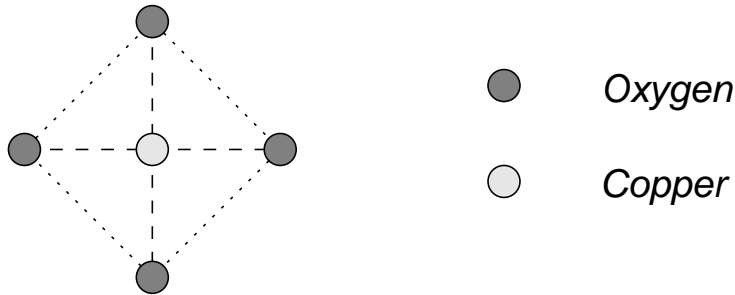


Figure 1. The topology of the CuO_4 cluster.

The smallest square Cu-O cluster, CuO_4 , see Fig. 1, is also the simplest where $W = 0$ pairing occurs. The Hamiltonian reads:

$$H_{\text{CuO}_4} = t \sum_{i\sigma} (d_{i\sigma}^\dagger p_{i\sigma} + p_{i\sigma}^\dagger d_{i\sigma}) + t_{pp} \sum_{\langle ij \rangle, \sigma} p_{i,\sigma}^\dagger p_{j,\sigma} + U(n_{\uparrow}^{(d)} n_{\downarrow}^{(d)} + \sum_i n_{i\uparrow}^{(p)} n_{i\downarrow}^{(p)}). \quad (5)$$

The one-body levels and their symmetry labels are reported in Table 2. Labelling the Oxygen atomic sites by the numbers 1, 2, 3, 4, the diagonalizing creation operator are

given by

$$\begin{aligned}
c_{E_y\sigma}^\dagger &= \frac{1}{\sqrt{2}} (p_{2\sigma}^\dagger - p_{4\sigma}^\dagger) \\
c_{E_x\sigma}^\dagger &= \frac{1}{\sqrt{2}} (p_{1\sigma}^\dagger - p_{3\sigma}^\dagger) \\
c_{B_1\sigma}^\dagger &= \frac{1}{2} (p_{1\sigma}^\dagger - p_{2\sigma}^\dagger + p_{3\sigma}^\dagger - p_{4\sigma}^\dagger) \\
c_{A_1\sigma}^\dagger(1) &= \frac{1}{\alpha_+^2 + 4} (\alpha_+ d_\sigma^\dagger + p_{1\sigma}^\dagger + p_{2\sigma}^\dagger + p_{3\sigma}^\dagger + p_{4\sigma}^\dagger) \\
c_{A_1\sigma}^\dagger(2) &= \frac{1}{\alpha_-^2 + 4} (\alpha_- d_\sigma^\dagger + p_{1\sigma}^\dagger + p_{2\sigma}^\dagger + p_{3\sigma}^\dagger + p_{4\sigma}^\dagger)
\end{aligned} \tag{6}$$

where α and β depend on $\tau = t_{pp}/t$ as follows

$$\alpha_\pm = \frac{4 \left(\pm 1 \pm \tau^2 + \tau \sqrt{4 + \tau^2} \right)}{\pm 5 \tau \pm 2 \tau^3 + \sqrt{4 + \tau^2} + 2 \tau^2 \sqrt{4 + \tau^2}}.$$

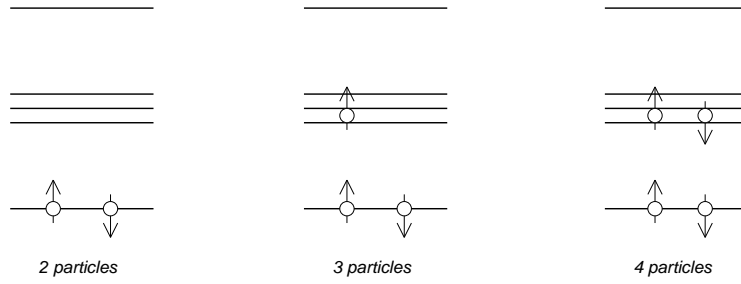


Figure 2. Many body states for the CuO_4 cluster. For each number of particle, it has been reported the component of highest weight of the ground state.

Let us build a 4-hole state in the CuO_4 cluster in the non-interacting limit, according to the *aufbau* principle, see Fig.2. The first two holes go into a bonding level of A_1 symmetry; this is a totally symmetric (1A_1) pair. For negative τ , the other two holes go into a non-bonding level of $E(x, y)$ symmetry, which contains 4 spin-orbital states. The Pauli principle allows $\binom{4}{2} = 6$ different pair-states. The irreducible multiplication table allows for labelling them according with their space symmetry: $E \otimes E = A_1 \oplus A_2 \oplus B_1 \oplus B_2$. It is also straightforward to verify that A_2 is a spin-triplet, 3A_2 , while the remaining irreps are spin-singlets, 1A_1 , 1B_1 and 1B_2 . From Eq. (6) one readily realize that the B_2 singlet operator

$$b_{B_2}^\dagger = \frac{1}{\sqrt{2}} (c_{E_x\uparrow}^\dagger c_{E_y\downarrow}^\dagger + c_{E_y\uparrow}^\dagger c_{E_x\downarrow}^\dagger) \tag{7}$$

is a $W = 0$ pair (no double occupation). Note that 1B_2 is the symmetry label of the pair wave function in the gauge we are using, and must not be confused with the symmetry of the order parameter.

To first order in perturbation theory, the 4-body singlet state of B_2 symmetry is degenerate with the A_2 triplet; Hund's rule would have predicted a 3A_2 ground state.

However, the true ground state turns out to be singlet, for reasons that we shall study below. The numerical results on the CuO_4 cluster show that $\tilde{\Delta}(4)$ is negative for $0 > \tau > -0.5$ and that its minimum value occurs at $\tau = 0$, when the non-bonding orbitals B_1 and E become degenerate: the paired interacting ground state is also degenerate in this particular case. A symmetry analysis of this accidental degeneracy is postponed to the next Section. In Fig. 3 we plot $\tilde{\Delta}(4)$ for $\tau = 0$, $\varepsilon_p - \varepsilon_d = 0$, $U_{pd} = 0$ and $U_p = U_d = U$. $\tilde{\Delta}(4)$ has a minimum at $U \approx 5 t$ and it is negative when

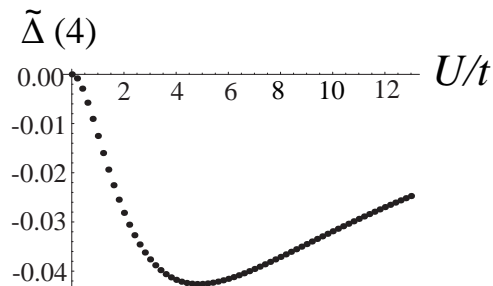


Figure 3. $\tilde{\Delta}(4)$ (in t units) as a function of U/t . The maximum binding occurs at $U \sim 5t$ where $\tilde{\Delta}(4) \approx -0.042 t$. For $U > 34.77 t$ (not shown), $\tilde{\Delta}(4)$ becomes positive and pairing disappears.

$0 < U < 34.77 t$. We emphasize that $\tilde{\Delta}(4)$ becomes positive for large values of U/t and hence pairing disappears in the strong coupling regime. In the present problem U must exceed several tens of times t before the asymptotic *strong coupling regime* sets in. A perturbation theory will strictly apply at *weak coupling* where the second derivative of the curve is negative. However, qualitatively a weak coupling approach is rewarding in all the physically interesting range of parameters. The sign of $\tilde{\Delta}$ depends on U and τ and its magnitude is unlike any of the input parameters; below we show that this new energy scale comes out from an interference between electron-hole exchanges of different symmetries.

On the other hand, at positive τ 's the B_1 non-bonding level is pushed below the degenerate one and $\tilde{\Delta}(4)$ becomes large and positive (at $\tau = +0.65$, $\tilde{\Delta}(4) = 0.53$ eV).

Next, we discuss the dependence of $\tilde{\Delta}(4)$ on the other parameters[34]. If we decrease ε_p , $\tilde{\Delta}(4)$ decreases because this makes the system more polarizable. The ε_p dependence when all the other parameter are kept fixed and $U_{pd} = 0$ is almost linear down to $\varepsilon_p = 0$. According to Ref.[30] positive U_{pd} values do not spoil the mechanism, and tend to be synergic with it. Indeed, values of $U_{pd} > 0.6$ eV give negative $\tilde{\Delta}(4)$ values even for $\tau = -0.65$ eV (in the range 0.2-1.2 eV considered in Ref.[34] $\tilde{\Delta}(4)$ is a monotonically decreasing function of U_{pd}). Finally, we have numerically studied how the distortions effect $\tilde{\Delta}(4)$. We have found that any lowering of the symmetry is reflected by a corresponding increase of $\tilde{\Delta}(4)$ [34].

In the CuO_4 cluster we need four holes to have a paired ground state. Hence, the total hole concentration is $\rho_h = 0.8$. This value is too large by a factor of 2 with

respect to the experimentally observed $\rho_h \simeq 0.4$ of the optimally doped systems. It is important to realize that these undesirable features are peculiar of the prototype CuO_4 cluster, and already disappear in Cu_5O_4 , the next larger cluster of the same symmetry. In fact, four holes are still sufficient to reach degenerate states, but $\rho_h \sim 0.44$ is much closer to the experimental value. We have performed numerical explorations in other fully symmetric clusters like Cu_5O_4 and Cu_5O_{16} and we have found negative values of $\tilde{\Delta}(4)$, of the order of few meV, using physical parameters. In all the allowed clusters up to 21 atoms, the lowest one-hole level belongs to A_1 symmetry, and the next E level yields the $W = 0$ pair. The interactions produce a non-degenerate 1B_2 4-hole ground state *having the same symmetry as the $W = 0$ pair*. The interested reader may see Refs.[43],[44] for the details. Below, in Section 3 we show[45] that the $\tilde{\Delta}(4) < 0$ arises from an effective attractive interaction between the holes of the $W = 0$ pair; the same interaction is repulsive for triplet pairs.

2.2. Symmetry of the $W = 0$ pairs: a general theorem

Since the mechanism depends on symmetry in such a fundamental way, we must refine the Group Theory analysis. We discovered a powerful and elegant criterion[46] to construct all the $W = 0$ pair eigenstates on a given lattice Λ by using projection operators.

Let \mathcal{G}_0 be the the symmetry Group of the non-interacting Hubbard Hamiltonian $K = \sum_{\langle ij \rangle, \sigma} t_{ij} c_{j\sigma}^\dagger c_{i\sigma}$. We assume that no degeneracy between one-body eigenstates is accidental, hence \mathcal{G}_0 must contain enough operations to justify all such degeneracies. Let us label each one-body eigenstate of $H = K + W$, $W = \sum_{i \in \Lambda} U_i n_{i\uparrow} n_{i\downarrow}$, with an irreducible representation (irrep) of \mathcal{G}_0 .

Definition. An irrep η is represented in the one-body spectrum of H if at least one of the one-body levels belongs to η .

Let \mathcal{E} be the set of the irreps of \mathcal{G}_0 which are represented in the one-body spectrum of H . Let $|\psi\rangle$ be a two-body eigenstate of the non-interacting Hamiltonian with spin $S^z = 0$ and $P^{(\eta)}$ the projection operator on the irrep η . We wish to prove the

$W = 0$ Theorem. - Any nonvanishing projection of $|\psi\rangle$ on an irrep not contained in \mathcal{E} , is an eigenstate of H with no double occupancy. The singlet component of this state is a $W = 0$ pair. Conversely, any pair belonging to an irrep represented in the spectrum must have non-vanishing W expectation value, see Fig. (4):

$$\eta \notin \mathcal{E} \Leftrightarrow WP^{(\eta)}|\psi\rangle = 0. \quad (8)$$

Remark: Suppose we perform a gauge change in H such that \mathcal{G}_0 is preserved; clearly, a $W = 0$ pair goes to another $W = 0$ pair. Thus, the theorem implies a distinction between symmetry types which is gauge-independent.

Proof: Let us consider a two-body state of opposite spins belonging to the irrep η of \mathcal{G}_0 :

$$|\psi^{(\eta)}\rangle = \sum_{ij \in \Lambda} \psi^{(\eta)}(i, j) c_{i\uparrow}^\dagger c_{j\downarrow}^\dagger |0\rangle.$$

Then we have

$$n_{i\uparrow} n_{i\downarrow} |\psi^{(\eta)}\rangle = \psi^{(\eta)}(i, i) c_{i\uparrow}^\dagger c_{i\downarrow}^\dagger |0\rangle \equiv \psi^{(\eta)}(i, i) |i \uparrow, i \downarrow\rangle.$$

We define $P^{(\eta)}$ as the projection operator on the irrep η . Since

$$P^{(\eta)} \sum_{i \in \Lambda} \psi^{(\eta)}(i, i) |i \uparrow, i \downarrow\rangle = \sum_{i \in \Lambda} \psi^{(\eta)}(i, i) |i \uparrow, i \downarrow\rangle,$$

if $P^{(\eta)} |i \uparrow, i \downarrow\rangle = 0 \ \forall i \in \Lambda$, then $\psi^{(\eta)}(i, i) = 0 \ \forall i \in \Lambda$. It is worth to note that this condition is satisfied if and only if $P^{(\eta)} |i\sigma\rangle = 0 \ \forall i \in \Lambda$, where $|i\sigma\rangle = c_{i\sigma}^\dagger |0\rangle$. Now it is always possible to write $|i\sigma\rangle$ in the form $|i\sigma\rangle = \sum_{\eta \in \mathcal{E}} c^{(\eta)}(i) |\eta_\sigma\rangle$ where $|\eta_\sigma\rangle$ is the one-body eigenstate of H with spin σ belonging to the irrep η . Hence, if $\eta' \notin \mathcal{E}$, $P^{(\eta')} |i\sigma\rangle = 0$ and so $P^{(\eta')} |i \uparrow, i \downarrow\rangle = 0$. Therefore, if $|\psi^{(\eta)}\rangle$ is a two-hole singlet eigenstate of the kinetic term and $\eta \notin \mathcal{E}$, then it is also an eigenstate of W with vanishing eigenvalue, that means a $W = 0$ pair.

Q.E.D.

The content of the theorem is schematically represented by Fig. (4).

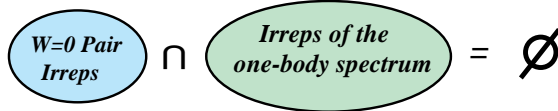


Figure 4. Schematic of the $W = 0$ theorem.

We already know that CuO_4 is a good example of this theorem. Indeed, the irrep B_2 of the $W = 0$ pair is not represented in the spectrum (see Table 2); A_2 is also not represented, but it yields no two-body states. This possibility is admitted by Eq. (8).

The particular case of CuO_4 with $\tau = 0$ is of special interest as an illustration. There is an *accidental* degeneracy between $E(x, y)$ and B_1 orbitals and therefore a three-times degenerate one-body level exists. With 4 interacting fermions, pairing occurs in two ways, as A_1 and B_2 are both degenerate ground states. This agrees with the theorem; in fact, the extra degeneracy cannot be explained in terms of C_{4v} , whose irreps have dimension 2 at most. For $\tau = 0$ any permutation of the four Oxygen sites is actually a symmetry and therefore \mathcal{G}_0 is enlarged to S_4 (the group of permutations of four objects). S_4 has the irreducible representations \mathcal{A}_1 (total-symmetric), \mathcal{B}_2 (total-antisymmetric), \mathcal{E} (self-dual), \mathcal{T}_1 and its dual \mathcal{T}_2 , of dimensions 1, 1, 2, 3 and 3, respectively. These irreps break in C_{4v} as follows

$$\mathcal{A}_1 = A_1, \quad \mathcal{T}_1 = B_1 \oplus E, \quad \mathcal{T}_2 = A_2 \oplus E, \quad \mathcal{B}_2 = B_2, \quad \mathcal{E} = A_1 \oplus B_2.$$

Labelling the one-body levels with the irreps of S_4 , one finds that \mathcal{E} is not contained in the spectrum and thus yields $W = 0$ pairs:

$${}^1\mathcal{E} = {}^1A_1 \oplus {}^1B_2. \quad (9)$$

The explicit expression of the corresponding pair-creation operators is

$$b_{A_1}^\dagger = \frac{2}{\sqrt{3}} c_{B_1\uparrow}^\dagger c_{B_1\downarrow}^\dagger + \frac{1}{\sqrt{3}} (c_{E_x\uparrow}^\dagger c_{E_x\downarrow}^\dagger + c_{E_y\uparrow}^\dagger c_{E_y\downarrow}^\dagger)$$

for the total-symmetric pair and Eq. (7) for the B_2 component.

In Section 4.3 we shall show use the theorem with a \mathcal{G}_0 that includes symmetries which are not isometries. We shall see that this theorem puts useful restrictions on the many-body ground state symmetry. The complete characterization of the symmetry of $W = 0$ pairs requires the knowledge of \mathcal{G}_0 . A partial use of the theorem is possible if one does not know \mathcal{G}_0 but knows a Subgroup $\mathcal{G}_0^<$. It is then still granted that any pair belonging to an irrep of $\mathcal{G}_0^<$ not represented in the spectrum has the $W = 0$ property. On the other hand, accidental degeneracies occur with a Subgroup of \mathcal{G}_0 , and by mixing degenerate pairs belonging to irreps represented in the spectrum one can find $W = 0$ pairs also there.

The theorem tells us that the *bigger* is \mathcal{G}_0 , the *larger* is the number of $W = 0$ pairs. Indeed, for a given system, the number of one-body eigenvectors is fixed, while the number and the dimension of the irreps grow with the order of the group. Therefore, also the number of irreps not represented in \mathcal{E} grows, meaning more $W = 0$ pairs. At the same time, a big “non-interacting” symmetry Group \mathcal{G}_0 grants large level degeneracies. As we have seen, this fact allows the existence of $W = 0$ pairs formed by degenerate orbitals. In the next Section we show that an anomalously low effective repulsion takes place in the interacting system when such levels are on the Fermi surface and that in a certain region of the parameters space this leads to pairing.

3. Theory of Pairing in repulsive Hubbard Models

In Section 2 we have shown that $W = 0$ pairs may lead to a paired ground state in fully symmetric C_{4v} clusters centered around a Cu ion. In this Section we extend the theory to the full plane, and show that such pairs provide the natural explanation of the pairing instability of the Hubbard Model. By a novel canonical transformation approach, we shall calculate the effective interaction W_{eff} between two holes added to the ground state of the repulsive Hubbard Model. Furthermore, we shall show that W_{eff} is attractive in the $W = 0$ pair-symmetry channels. The method is a particularly efficient way to perform the configuration interaction calculation. It is based on the symmetry and sheds light on the origin of pairing in the CuO_2 plane. It is worth noticing that $W = 0$ pairs emerge from symmetry alone and hence remain $W = 0$ for any coupling strength U . This is the reason why weak coupling expansions provide often good approximations at intermediate coupling as well, as observed by several authors[47],[48],[49].

3.1. $W = 0$ Pairs in the Planar Hubbard Model

The CuO_2 planes of cuprates have a large symmetry group which contains the space group $\mathcal{G} = T \otimes C_{4v}$, where T is the group of translations and \otimes stands for the semidirect product. However, the Optimal Group \mathcal{G}_0 is much larger than \mathcal{G} [50]. For this reason, instead of using the $W = 0$ theorem, it is easier to follow the simple route of projecting a single determinantal state on the irreps of C_{4v} [51],[52]. This partial use of the symmetry still gives enough solutions to demonstrate pairing.

Let us focus on $W = 0$ pairs with vanishing quasimomentum. Omitting band indices, we denote by

$$|d[\mathbf{k}]\rangle = c_{\mathbf{k},\uparrow}^\dagger c_{-\mathbf{k},\downarrow}^\dagger |0\rangle \quad (10)$$

a two-hole determinantal state, where \mathbf{k} and $-\mathbf{k}$ label degenerate one-body eigenfunctions of K . The combination $|d[\mathbf{k}]\rangle + |d[-\mathbf{k}]\rangle$ is singlet and $|d[\mathbf{k}]\rangle - |d[-\mathbf{k}]\rangle$ is triplet. We introduce the determinants $|d[R\mathbf{k}]\rangle \equiv |d[\mathbf{k}_R]\rangle$, $R \in C_{4v}$, and the projected states

$$|\Phi_\eta[\mathbf{k}]\rangle = \frac{1}{\sqrt{8}} \sum_{R \in C_{4v}} \chi^{(\eta)}(R) |d[\mathbf{k}_R]\rangle \quad (11)$$

where $\chi^{(\eta)}(R)$ is the character of the operation R in the irrep η .

In the Three Band Model we showed that $W = 0$ pairs are obtained by projecting onto the irreps A_2 and B_2 [53] (which are not represented in the one-body spectrum, as it should). These irreps differ by those obtained in the fully symmetric clusters, where $W = 0$ pairs had A_1 and B_2 symmetry[54]. The reason for this change is a twofold size effect. On one hand, A_1 pairs have the $W = 0$ property only in clusters having the topology of a cross (whose symmetry group is S_4 rather than C_{4v}), but do not generalize as such to the full plane (when the symmetry is lowered to C_{4v}). On the other hand, the small clusters admit no $W = 0$ solutions of A_2 symmetry if only degenerate states are used.

We recall that a necessary condition for pairing in clusters is that the least bound holes form a $W = 0$ pair, and this dictates conditions on the occupation number. In the full plane, however, $W = 0$ pairs exist at the Fermi level for any filling. We also observe that the $W = 0$ pairs obtained with the above procedure are not *all* the possible $W = 0$ pairs in the One and Three Bands Hubbard models, since the $W = 0$ theorem has not been fully exploited. However, it can be shown that they are the only $W = 0$ pairs with holes in degenerate one-body levels and with vanishing quasimomentum.

3.2. Canonical Transformation

In this Section we intend to study the effective interaction W_{eff} between the particles forming a $W = 0$ pair added to the N -body interacting ground state $|\Phi_U(N)\rangle$. Since the two extra particles cannot interact directly (by definition of $W = 0$ pair), their effective interaction comes out from virtual electron-hole exchanges, and in principle can be attractive.

Many configurations contribute to the interacting $(N + 2)$ -body ground state $|\Phi_U(N + 2)\rangle$ and we need a complete set \mathcal{S} to expand it exactly; as long as it is complete, however, we can design \mathcal{S} as we please. We can take the non-interacting N -body Fermi sphere $|\Phi_0(N)\rangle$ as our vacuum and build the complete set in terms of excitations over it. In the subspace with vanishing spin z component, the simplest states that enter the configuration mixing are those obtained from $|\Phi_0(N)\rangle$ by creating two extra holes[55] over it; we denote with $|m\rangle$ these states. Similarly, along with the pair m states, we introduce the 4-body α states, obtained from $|\Phi_0(N)\rangle$ by creating 2 holes and 1 electron-hole (e-h) pair. Then, \mathcal{S} includes the 6-body β states having 2 holes and 2 e-h pairs, and so on. We are using Greek indices for the configurations containing the electron-hole pairs, which here are playing largely the same role as phonons in the Cooper theory. By means of the complete set \mathcal{S} we now expand the interacting ground state

$$|\Phi_U(N + 2)\rangle = \sum_m a_m |m\rangle + \sum_\alpha a_\alpha |\alpha\rangle + \sum_\beta a_\beta |\beta\rangle + \dots \quad (12)$$

and set up the Schrödinger equation

$$H|\Phi_U(N + 2)\rangle = E|\Phi_U(N + 2)\rangle.$$

We emphasize that Eq. (12) is a configuration interaction, *not a perturbative expansion*. When the number N of holes in the system is such that $|\Phi_0(N)\rangle$ is a single non-degenerate determinant (the Fermi surface is totally filled), the expansion (12) for the interacting ground state is unique and we can unambiguously define and calculate the effective interaction W_{eff} . This is done by a canonical transformation[44],[51],[52] of the many-body Hubbard Hamiltonian. We consider the effects of the operators K and W on the terms of $|\Phi_U(N + 2)\rangle$. Choosing the m , α , β , \dots states to be eigenstates of the kinetic operator K , we have

$$K|m\rangle = E_m|m\rangle, \quad K|\alpha\rangle = E_\alpha|\alpha\rangle, \quad K|\beta\rangle = E_\beta|\beta\rangle, \quad \dots$$

The Hubbard interaction W can create or destroy up to 2 e-h pairs. Therefore, its action on an m state yields

$$W|m\rangle = \sum_{m'} W_{m',m}|m'\rangle + \sum_\alpha W_{\alpha,m}|\alpha\rangle + \sum_\beta W_{\beta,m}|\beta\rangle,$$

on an α states yields

$$W|\alpha\rangle = \sum_m W_{m,\alpha}|m\rangle + \sum_{\alpha'} W_{\alpha',\alpha}|\alpha'\rangle + \sum_\beta W_{\beta,\alpha}|\beta\rangle + \sum_\gamma W_{\gamma,\alpha}|\gamma\rangle,$$

and so on. In this way we obtain an algebraic system for the coefficients of the configuration interaction of Eq. (12). In order to test the instability of the Fermi liquid towards pairing, it is sufficient to study the amplitudes a_m of the m states. In the weak coupling limit this can be done by truncating the expansion (12) to the α states. As we have shown[52], the inclusion of the β , γ , \dots states produces a E -dependent

renormalization of the matrix elements of higher order in W , leaving the structure of the equations unaltered.

By taking a linear combination of the α states in such a way that

$$(K + W)_{\alpha, \alpha'} = \delta_{\alpha \alpha'} E'_\alpha$$

the algebraic system reduces to

$$\begin{aligned} [E_m - E] a_m + \sum_{m'} W_{m, m'} a_{m'} + \sum_{\alpha} W_{m, \alpha} a_{\alpha} &= 0 \\ [E'_\alpha - E] a_{\alpha} + \sum_{m'} W_{\alpha, m'} a_{m'} &= 0. \end{aligned} \quad (13)$$

Solving for a_{α} and substituting back in Eq. (13), we end up with an equation for the dressed pair $|\psi\rangle \equiv \sum_m a_m |m\rangle$. The effective Schrödinger equation for the pair reads

$$(K + W + S[E]) |\psi\rangle \equiv H_{\text{pair}} |\psi\rangle = E |\psi\rangle \quad (14)$$

where

$$(S[E])_{m, m'} = - \sum_{\alpha} \frac{W_{m, \alpha} W_{\alpha, m'}}{E'_\alpha - E}. \quad (15)$$

is the scattering operator. The matrix elements $W_{m, m'}$ in Eq. (14) may be written as the sum of two terms representing the direct interaction $W_{m, m'}^{(d)}$ between the particles forming the pair and the first-order self-energy W_m :

$$W_{m, m'} = W_{m, m'}^{(d)} + \delta_{m, m'} W_m.$$

Similarly, in $S[E]$ we may recognize two different contributions; one is the true effective interaction W_{eff} , while the other is the forward scattering term F

$$S_{m, m'} = (W_{\text{eff}})_{m, m'} + F_m \delta_{m, m'}.$$

The first-order self-energy and the forward scattering term are diagonal in the indices m and m' . W_m and F_m renormalize the non-interacting energy E_m of the m states:

$$E_m \rightarrow E_m^{(R)} = E_m + W_m + F_m.$$

Eq. (14) has the form of a Schrödinger equation with eigenvalue E for the added pair with the interaction $W^{(d)} + W_{\text{eff}}$. Here, the $W = 0$ pairs are special because $W^{(d)}$ vanishes. We interpret a_m as the wave function of the dressed pair, which is acted upon by an effective Hamiltonian H_{pair} . This way of looking at Eq. (14) is perfectly consistent, despite the presence of the many-body eigenvalue E . Indeed, if the interaction is attractive and produces bound states, the spectrum contains discrete states below the threshold of the continuum (two-electron Fermi energy). This is a clear-cut criterion for pairing, which is exact in principle. The threshold is given by

$$E_F^{(R)} \equiv \min_{\{m\}} [E_m^{(R)}(E)],$$

and contains all the pairwise interactions except those between the particles in the pair. $E_F^{(R)}$ must be determined once Eq. (14) has been solved (since F depends on the solution). The ground state energy E may be conveniently written as $E_F^{(R)} + \Delta$. $\Delta < 0$ indicates a Cooper-like instability of the normal Fermi liquid and its magnitude represents the binding energy of the pair.

It is worth noticing that in principle the canonical transformation is exact and it is not limited to the weak coupling regime. In the numerical calculations, however, some approximation is needed. In practice, we shall compute the bare quantities, that is, we shall neglect the 6-body and higher excitations in the calculation of W_{eff} and F . This is a reasonable approximation if we compute small corrections to a Fermi liquid background, and the exact numerical results obtained in small clusters suggest that this is the case, see next Section.

3.3. Pairing in the CuO_4 Cluster

We defined the pairing energy for a cluster with $N + 2$ particles by introducing the quantity $\tilde{\Delta}(N+2) = E(N+2) + E(N) - 2E(N+1)$. At weak coupling we have shown in Ref.[45] that $\tilde{\Delta}$ agrees with the binding energy Δ obtained from many-body perturbation theory. Here, we consider again the CuO_4 cluster; we intend to test our canonical transformation by comparing the analytic results with the exact diagonalization data obtained in Section 2.

The CuO_4 cluster can host a $W = 0$ pair of B_2 symmetry. At weak coupling, we can ignore the effect of the renormalizations in Eq. (15). Furthermore, we can discard the inter-shell interactions. Indeed, the one-body levels of finite clusters are widely separated and the dominant contribution to the effective interaction comes from the intra-shell interaction. Accordingly, in Eq. (15) we set the $m = m' = B_2$. The one-body levels and their symmetry labels are reported in Table 2.

The effective interaction in the B_2 symmetry channel is

$$W_{\text{eff}}^{(B_2)} \equiv \sum_{\alpha} \frac{W_{B_2,\alpha} W_{\alpha,B_2}}{E_{\alpha} - E} = -\frac{U^2}{32} \left[\frac{2}{\varepsilon_{B_1} + \varepsilon_{A_1} - E} - \frac{1}{\varepsilon_{A'_1} + \varepsilon_{A_1} - E} \right].$$

The binding energy is obtained by expressing the lowest eigenvalue E of H_{pair} as $E = E_F^{(R)} + \Delta$. The renormalized two-hole Fermi energy $E_F^{(R)}$ coincides with the bare one at this level of accuracy, *i.e.*, $E_F^{(R)} = 2\varepsilon_{A_1}$. The results are shown in Fig. 5 for $\tau = 0$. We can see that Δ is negative and hence the renormalization approach predicts pairing, at least at weak coupling. We also observe that the order of magnitude of $|\Delta|$ is $10^{-2}t$, which is not comparable to any of the U and t input parameters. The reason is that the interaction, which vanishes identically for the *bare* $W = 0$ pairs, remains *dynamically* small for the dressed quasiparticles. This suggests that a *weak coupling* theory may be useful to study the pairing force, despite the fact that U is not small compared to t .

Next, we intend to compare Δ with the quantity $\tilde{\Delta}(4)$ obtained from exact diagonalizations, see Fig. 3. At weak coupling the agreement is excellent. However,

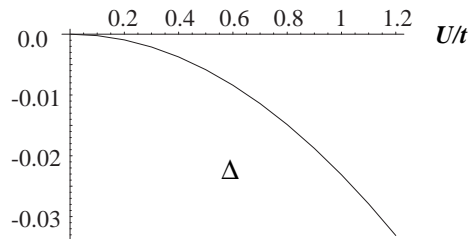


Figure 5. Trend of Δ versus U/t in units of t .

$|\Delta|$ is ~ 2 times greater than $|\tilde{\Delta}(4)|$ for $U/t \simeq 1$. This means that the inter-shell interactions and the renormalizations of the α -state energies have an important weight in determining the right value of Δ . However, what is comfortable is that the analytic approach predicts the right trend of the binding energy. In the next Section we shall use the canonical transformation to study larger and more physical systems.

3.4. Pairing in the CuO_2 Plane: Numerical Results

Using the analytic expression for the effective interaction in the full plane, we have performed exploratory numerical estimates of Δ by working on supercells of $N_\Lambda \times N_\Lambda$ cells, with periodic boundary conditions. For the sake of simplicity, we have neglected the minor contributions from the higher bands and considered the dominant intra-band processes, in which empty states belong to the bonding band. We have solved the problem in a virtually exact way for N_Λ up to 40. Several supercell calculations had been reported to date[9], but no conclusive evidence of a pairing instability was reached due to the difficulty of dealing with size effects.

First, we have investigated triplet pairing but, as in the clusters, we have found a repulsive effective interaction. On the contrary, $W = 0$ singlets show pairing, in line with our previous findings in small clusters[34],[43],[45]. Since screening excitations are explicitly accounted for in the Hamiltonian, it is likely that U is a bare (unscreened) quantity, which justify large values. A stronger interaction causes smaller pairs and speeds up convergence within attainable supercell sizes. In Table 3, we report the results for 1B_2 pairs with $\varepsilon_F = -1.3$ eV [half filling corresponds to $\varepsilon_F = -1.384$ eV and we have used as input data the set of current parameters already used for clusters, that is (in eV) $t = 1.3$, $\varepsilon_p = 3.5$, $\varepsilon_d = 0$, $U_p = 12.5$, $U_d = 11.2$].

With supercell sizes $N_\Lambda > 40$ calculations become hard. Thus, we need a simple solvable model in supercells and in the infinite plane to make reliable extrapolations of numerical results. To this end, we introduce an Average Effective Interaction (AEI) $-V_{\text{eff}}$, $V_{\text{eff}} > 0$, which is constant for all the empty states \mathbf{k} and \mathbf{k}' . For any N_Λ , V_{eff} is implicitly defined from

$$\frac{8}{V_{\text{eff}}} = \frac{1}{N_\Lambda^2} \sum_{\mathbf{k}} \frac{\theta(\varepsilon_{\mathbf{k}} - \varepsilon_F)}{2(\varepsilon_{\mathbf{k}} - \varepsilon_F) + |\Delta|},$$

(the factor 8 comes from the projection onto the irrep B_2). Although $|\Delta|$ decreases monotonically by increasing N_Λ , V_{eff} remains fairly stable around $6 \div 7$ eV, see Table 3.

N_Λ	$\rho = N/N_\Lambda^2$	$-\Delta$ (meV)	V_{eff} (eV)	$-\Delta_{\text{asympt}}$ (meV)
18	1.13	121.9	7.8	41.6
20	1.16	42.2	5.0	9.0
24	1.14	59.7	7.0	28.9
30	1.14	56.0	5.7	13.2
40	1.16	30.5	6.6	23.4

Table 3. Binding energy of 1B_2 pairs in supercells.

The relatively mild N_Λ dependence of V_{eff} supports the use of the AEI to extrapolate the results to the thermodynamic limit. The asymptotic value $\lim_{N_\Lambda \rightarrow \infty} |\Delta| \equiv \Delta_{\text{asympt}}$ can then be obtained from

$$\frac{8}{V_{\text{eff}}} = \int_{\varepsilon_F}^0 \frac{d\varepsilon \rho(\varepsilon)}{2(\varepsilon - \varepsilon_F) + |\Delta_{\text{asympt}}|},$$

where ρ is the density of states.

The results for the 1A_2 pairs are seen to lead to bound states as well, with comparable Δ values[51]; the trend with doping is opposite, however, and the binding energy is nearly closing at $\varepsilon_F = -1.1$ eV.

Although the three-band Hubbard Model is an idealization of the strongly correlated CuO_2 planes, it is interesting to observe that evidence of mixed ($s + id$) symmetry for the pairing state has been amply reported in angle-resolved photoemission studies[56],[57].

4. The Doped Hubbard Antiferromagnet

The canonical transformation described in Section 3.2 relies on the uniqueness of the non-interacting ground state $|\Phi_0(N)\rangle$. $|\Phi_0(N)\rangle$ is certainly unique if the Fermi surface is totally filled and it can be written as a Slater determinant. However, we are also particularly interested in the doped Hubbard antiferromagnet, and the antiferromagnetic ground state occurs at half filling, *not* in a filled-shell situation.

We want to study the doped antiferromagnet since there are strong indications that the Fermi liquid is unstable towards pairing near half filling; they come from diagrammatic approaches[15], renormalization group techniques[16],[17] and also cluster diagonalizations[32]. Therefore exact results on the half filled Hubbard Model may be relevant to antiferromagnetism and to the mechanism of the superconducting instability as well. The Lieb theorem[25] on the ground state spin-degeneracy of the half-filled Hubbard model ensures that for any bipartite lattice $\Lambda = \mathcal{A} \cup \mathcal{B}$, with $|\mathcal{A}| = |\mathcal{B}|$, the ground state is unique for any interaction strength U . Thus, we can use the canonical transformation with $|\Phi_0(N)\rangle = \lim_{U \rightarrow 0^+} |\Phi_U(N)\rangle$ provided the number of holes N equals the number of sites $|\Lambda|$. Remarkably, the $W = 0$ pairs are also essential tools to deal with the antiferromagnetic ground state solution. Below, we present two exact results.

First, we obtain the ground state $|\Phi_U(|\Lambda|)\rangle$ on the so called *complete bipartite graph* (CBG) for arbitrary but finite U . Then, we consider the square lattice and we resolve the degeneracy of the non-interacting ground-state multiplet at half filling. This latter result will then be used to study the pairing mechanism in the 4×4 Hubbard model.

4.1. Half-Filled Hubbard Model on the Complete Bipartite Graph

The Complete Bipartite Graph (CBG) $\Lambda = \mathcal{A} \cup \mathcal{B}$ has bonds connecting any element of \mathcal{A} with all the elements of \mathcal{B} . In Fig. 6 we have drawn a few examples of finite-size systems. For $N = 1$ and $N = 2$ the model is equivalent to a one dimensional ring of length $L = 2, 4$ respectively. For $N = 3$ we have what can be understood as a prototype, (1,1) *nanotube* model, the one of smallest length $L = 1$, with periodic boundary conditions. For general N , one can conceive a *gedanken* device, like the one illustrated pictorially for $N = 6$ in Fig. 6.d. The N vertical lines represent a realization of the \mathcal{A} sublattice while the \mathcal{B} sublattice is mimicked by the central object. The radial tracks in the Figure represent conducting paths linking each \mathcal{A} site to each \mathcal{B} site according to the topology of our model.

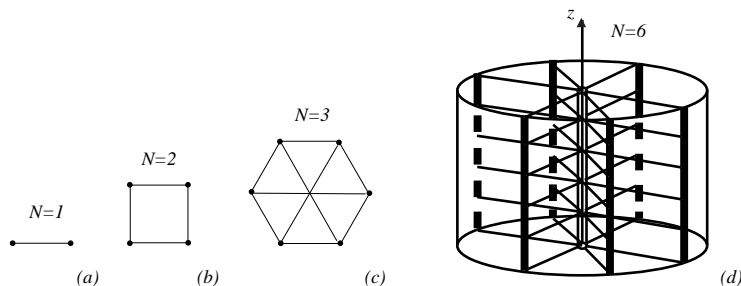


Figure 6. Physical representation of the CBG for $N = 1$ (a) and $N = 2$ (b) which is equivalent to a one dimensional ring of length $L = 2, 4$ respectively. For $N = 3$ (c) we have the (1,1) nanotube of smallest length and periodic boundary conditions. For $N = 6$ (d) we present the *gedanken* device described in the text.

Our solution is an example of *antiferromagnetic* ground state in a model of itinerant electrons; it may provide useful hints about antiferromagnetism outside the strong coupling regime (where the Hubbard model can be mapped onto the Heisenberg model).

The model is invariant under an arbitrary permutation of the \mathcal{A} -sites and/or of the \mathcal{B} -sites. In the symmetric case $|\mathcal{A}| = |\mathcal{B}|$ there is an additional Z_2 symmetry because of the $\mathcal{A} \leftrightarrow \mathcal{B}$ exchange. In what follows we shall focus on the symmetric case and we call \mathcal{N} the number of sites in each sublattice, $|\Lambda| = 2\mathcal{N}$.

The one-body spectrum has three different eigenvalues $\varepsilon_g = -t$, $\varepsilon_0 = 0$ and $\varepsilon_{\bar{g}} = t$ with degeneracy $d_g = 1$, $d_0 = 2\mathcal{N} - 2$ and $d_{\bar{g}} = 1$ respectively. We use the convention $t > 0$ so that ε_g is the lowest level and we shall call \mathcal{S}_{hf} the set of zero-energy one-body eigenstates, $|\mathcal{S}_{hf}| = 2\mathcal{N} - 2$. The zero-energy one-body orbitals can be visualized by a simple argument. Consider any pair i, j , with $i \neq j$, of sites belonging to the same

sublattice, say \mathcal{A} , and a wavefunction $\psi_{i,j}$ taking the values 1 and -1 on the pair and 0 elsewhere in \mathcal{A} and in \mathcal{B} . It is evident that $\psi_{i,j}$ belongs to \mathcal{S}_{hf} . Operating on $\psi_{i,j}$ by the permutations of $S_{\mathcal{N}}$ we can generate a (non-orthogonal) basis of $\mathcal{N} - 1$ eigenfunctions vanishing in \mathcal{B} ; further, by means of the Z_2 symmetry, we obtain the remaining orbitals of \mathcal{S}_{hf} , which vanish on \mathcal{A} . This exercise shows that the group considered above justifies the $(2\mathcal{N} - 2)$ -fold degeneracy of the one-body spectrum.

We denote by g (\bar{g}) the operator which annihilates a particle in the eigenstate with energy ε_g ($\varepsilon_{\bar{g}}$). Then, the kinetic term K can be written as

$$K = -t \sum_{\sigma} (g_{\sigma}^{\dagger} g_{\sigma} - \bar{g}_{\sigma}^{\dagger} \bar{g}_{\sigma}) .$$

Next, we introduce the one-body eigenstate $a_i^{\dagger}|0\rangle$ of \mathcal{S}_{hf} with vanishing amplitudes on the \mathcal{B} sublattice. Similarly, $b_i^{\dagger}|0\rangle$ has vanishing amplitude on the \mathcal{A} sublattice and therefore the $(2\mathcal{N} - 2)$ -body state

$$|\Phi_{AF}^{(\sigma)}\rangle = a_{1\sigma}^{\dagger} \dots a_{\mathcal{N}-1\sigma}^{\dagger} b_{1\bar{\sigma}}^{\dagger} \dots b_{\mathcal{N}-1\bar{\sigma}}^{\dagger} |0\rangle, \quad \bar{\sigma} = -\sigma \quad (16)$$

is an eigenstate of K and of W with vanishing eigenvalue. In the following we shall use the wording $W = 0$ state to denote any eigenstate of H in the kernel of W . It is worth noticing that by mapping the \mathcal{A} -sites onto the \mathcal{B} -sites and *viceversa*, $|\Phi_{AF}\rangle$ retains its form except for a spin-flip; we call this property the *antiferromagnetic property* for obvious reasons.

The state $|\Phi_{AF}\rangle$ plays a crucial role in building the exact ground state at half filling. We first observe that $|\Phi_{AF}\rangle$ has non-vanishing projection onto all the total spin subspaces $S = 0, \dots, \mathcal{N} - 1$. Let us denote with $|\Phi_{AF}^{0,0}\rangle$ the singlet component and with $|\Phi_{AF}^{1,m}\rangle$, $m = 0, \pm 1$, the triplet component. We further introduce the short-hand notation $|g^0\rangle \equiv g_{\uparrow}^{\dagger} g_{\downarrow}^{\dagger} |0\rangle$ and $|\bar{g}^0\rangle \equiv \bar{g}_{\uparrow}^{\dagger} \bar{g}_{\downarrow}^{\dagger} |0\rangle$ for the two-body singlets that one obtains from the lowest and the highest energy orbitals g and \bar{g} , and $[[g\bar{g}]^{1,m}\rangle$, $m = 0, \pm 1$, for the corresponding triplet. Then, one can prove[58] that the interacting ground state $|\Phi_U(|\Lambda|)\rangle$ can be written as

$$|\Phi_U(|\Lambda|)\rangle = [\gamma_g |g^0\rangle + \gamma_{\bar{g}} |\bar{g}^0\rangle] \otimes |\Phi_{AF}^{0,0}\rangle + \gamma_0 \sum_{m=-1}^1 (-)^m [[g\bar{g}]^{1,m}\rangle \otimes |\Phi_{AF}^{1,-m}\rangle ,$$

where $(\gamma_g, \gamma_{\bar{g}}, \gamma_0)$ is the lowest energy eigenvector of a 3×3 Hermitean matrix[58].

We observe that $|\Phi_U(|\Lambda|)\rangle$ is an eigenstate of the total number operator $\hat{n}^a + \hat{n}^b$ of particles in the shell \mathcal{S}_{hf} , despite the fact that $[\hat{n}^a + \hat{n}^b, H] \neq 0$. Such a remarkable property (*shell population rigidity*) relies on the cancellation of those scattering amplitudes that do not preserve the number of particles in \mathcal{S}_{hf} . We have shown[58] that this cancellation takes place provided in \mathcal{S}_{hf} the $(2\mathcal{N} - 2)$ -body state is a $W = 0$ state. We have also found that the ground state energy $E(|\Lambda|)$ is negative for any value of the repulsion U ; qualitatively, we may say that the particles manage to avoid the double occupation very effectively. Furthermore, $E(|\Lambda|)$ is a monotonically increasing function of U and \mathcal{N} due to the existence of non-trivial correlations even

for large \mathcal{N} . The nature of these correlations has been investigated by computing the expectation value of the repulsion. We have shown that for any finite \mathcal{N} there is a critical value of U yielding maximum repulsion. Even more interesting is the magnetic order of the ground state. Due to the $S_{\mathcal{N}} \otimes S_{\mathcal{N}} \otimes Z_2$ symmetry, the spin-spin correlation function $G_{\text{spin}}(i, j) \equiv \langle \Phi_U(|\Lambda|) | S_i^z S_j^z | \Phi_U(|\Lambda|) \rangle$ can be written as

$$G_{\text{spin}}(i, j) = \begin{cases} G_0 & i = j \\ G_{\text{on}} & i \in \mathcal{A} \text{ (} i \in \mathcal{B} \text{) and } j \in \mathcal{A} \text{ (} j \in \mathcal{B} \text{)} \\ G_{\text{off}} & i \in \mathcal{A} \text{ (} i \in \mathcal{B} \text{) and } j \in \mathcal{B} \text{ (} j \in \mathcal{A} \text{)} \end{cases}$$

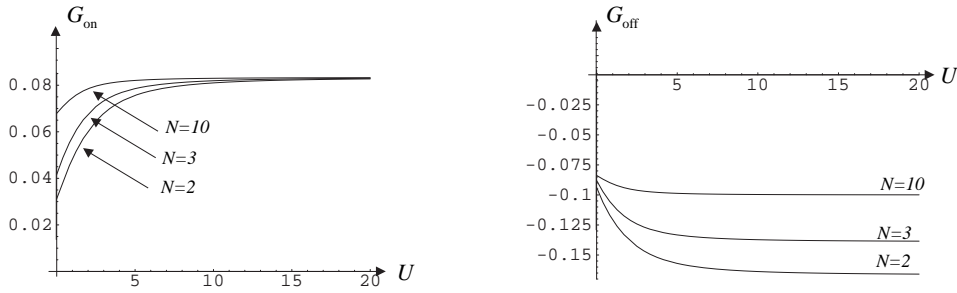


Figure 7. a) G_{on} versus U in the range $0 \leq U \leq 20$ for three different values of the number of sites $\mathcal{N} = 2, 3, 10$. b) G_{off} versus U in the range $0 \leq U \leq 20$ for three different values of the number of sites $\mathcal{N} = 2, 3, 10$. The hopping parameter has been chosen to be $t = 1$ in both cases.

In Fig. 7 we report the trend of G_{on} and G_{off} versus U for three different values of $\mathcal{N} = 2, 3, 10$. According to the Shen-Qiu-Tian theorem[59], G_{on} is always larger than zero while G_{off} is always negative. Next, we consider the ground state average of the square of the staggered magnetization operator

$$m_{AF}^2 \equiv \frac{1}{|\Lambda|} \langle \Phi_U | [\sum_{i \in \Lambda} \epsilon(i) S_i^z]^2 | \Phi_U \rangle, \quad \epsilon(i) = 1, -1 \text{ for } i \in \mathcal{A}, \mathcal{B}. \quad (17)$$

The Shen-Qiu-Tian theorem implies that each term in the expansion of Eq. (17) is non-negative. We emphasize, however, that for $|\mathcal{A}| = |\mathcal{B}|$ this does not imply that m_{AF}^2 is an extensive quantity! Remarkably, in the CBG $m_{AF}^2 = G_0 + (\mathcal{N} - 1)G_{\text{on}} - \mathcal{N}G_{\text{off}}$ is extensive for any value of the on-site repulsion U and provide the first example of antiferromagnetic ground state in a model of itinerant electrons.

4.2. Half-Filled Hubbard Model on the Square Lattice for $U = 0^+$

We consider the Hubbard Hamiltonian on the square lattice

$$H = K + W = \frac{t}{2} \sum_{\langle \mathbf{r}, \mathbf{r}' \rangle \sigma} (c_{\mathbf{r}\sigma}^\dagger c_{\mathbf{r}'\sigma} + \text{h.c.}) + U \sum_{\mathbf{r}} n_{\mathbf{r}\uparrow} n_{\mathbf{r}\downarrow} \quad (18)$$

with $\mathbf{r} = (i_x, i_y)$, $i_x, i_y = 1, \dots, N_\Lambda$ and the sum on $\langle \mathbf{r}, \mathbf{r}' \rangle$ is over the pairs of nearest neighbors sites. The point symmetry is C_{4v} ; besides, H is invariant under

the commutative Group of translations \mathbf{T} and hence the space Group $\mathbf{G} = \mathbf{T} \otimes C_{4v}$; \otimes means the semidirect product. In terms of the Fourier expanded fermion operators (periodic boundary conditions) $c_{\mathbf{k}} = \frac{1}{N_{\Lambda}} \sum_{\mathbf{r}} e^{i\mathbf{k}\cdot\mathbf{r}} c_{\mathbf{r}}$, we have $K = \sum_{\mathbf{k}} \varepsilon_{\mathbf{k}} c_{\mathbf{k}\sigma}^{\dagger} c_{\mathbf{k}\sigma}$ with $\varepsilon_{\mathbf{k}} = 2t[\cos k_x + \cos k_y]$. Then, the one-body plane wave state $c_{\mathbf{k}\sigma}^{\dagger}|0\rangle \equiv |\mathbf{k}\sigma\rangle$ is an eigenstate of K .

In this Section we build the exact ground state of the Hubbard Hamiltonian (18) at half filling and weak coupling for a general *even* N_{Λ} . Once a unique non-interacting ground state is determined, one can use the non-perturbative canonical transformation to test the instability of the system towards pairing; this will be done in the next Section for $N_{\Lambda} = 4$.

The starting point is the following property of the number operator $n_{\mathbf{r}} = c_{\mathbf{r}}^{\dagger} c_{\mathbf{r}}$ (for the moment we omit the spin index).

Theorem: Let \mathcal{S} be an arbitrary set of plane-wave eigenstates $\{|\mathbf{k}_i\rangle\}$ of K and $(n_{\mathbf{r}})_{ij} = \langle \mathbf{k}_i | n_{\mathbf{r}} | \mathbf{k}_j \rangle = \frac{1}{N_{\Lambda}^2} e^{i(\mathbf{k}_i - \mathbf{k}_j) \cdot \mathbf{r}}$ the matrix of $n_{\mathbf{r}}$ in \mathcal{S} . This matrix has eigenvalues $\lambda_1 = \frac{|\mathcal{S}|}{N_{\Lambda}^2}$ and $\lambda_2 = \dots = \lambda_{|\mathcal{S}|} = 0$.

Note that $|\mathcal{S}| \leq N_{\Lambda}^2$; if $|\mathcal{S}| = N_{\Lambda}^2$ the set is complete, like the set of all orbitals, and the theorem is trivial (a particle on site \mathbf{r} is the $n_{\mathbf{r}}$ eigenstate with eigenvalue 1). Otherwise, if $|\mathcal{S}| < N_{\Lambda}^2$, the theorem is an immediate consequence of the fact[61] that

$$\det|(n_{\mathbf{r}})_{ij} - \lambda \delta_{ij}| = (-\lambda)^{|\mathcal{S}|-1} \left(\frac{|\mathcal{S}|}{N_{\Lambda}^2} - \lambda \right), \quad \forall \mathbf{r}. \quad (19)$$

Let \mathcal{S}_{hf} denote the set (or shell) of the \mathbf{k} wave vectors such that $\varepsilon_{\mathbf{k}} = 0$. At half filling (N_{Λ}^2 particles) for $U = 0$ the \mathcal{S}_{hf} shell is half occupied, while all \mathbf{k} orbitals such that $\varepsilon_{\mathbf{k}} < 0$ are filled. The \mathbf{k} vectors of \mathcal{S}_{hf} lie on the square having vertices $(\pm\pi, 0)$ and $(0, \pm\pi)$; one readily realizes that the dimension of the set \mathcal{S}_{hf} is $|\mathcal{S}_{hf}| = 2N_{\Lambda} - 2$. Since N_{Λ} is even and H commutes with the total spin operators, at half filling every ground state of K is represented in the $S^z = 0$ subspace. Thus, K has $\binom{2N_{\Lambda} - 2}{N_{\Lambda} - 1}^2$ degenerate unperturbed ground state configurations with $S^z = 0$. Most of the degeneracy is removed in first-order by W . We shall be able to single out the unique ground state of H by exploiting the Lieb theorem.

The first-order splitting of the degeneracy is obtained by diagonalizing the W matrix over the unperturbed basis; like in elementary atomic physics, the filled shells just produce a constant shift of all the eigenvalues and for the rest may be ignored in first-order calculations. In other terms we consider the *truncated Hilbert space* \mathcal{H} spanned by the *states of $N_{\Lambda} - 1$ holes of each spin in \mathcal{S}_{hf}* , and we want the *exact* ground state(s) of W in \mathcal{H} ; by construction \mathcal{H} is in the kernel of K , so the ground state of W is the ground state of H as well. Since the lowest eigenvalue of W is zero, it is evident that any $W = 0$ state in \mathcal{H} is a ground state of H .

To diagonalize the *local* operator W in closed form we need to set up a *local* basis set of one-body states. If \mathcal{S}_{hf} were the complete set of plane-wave states \mathbf{k} , the new basis would be trivially obtained by a Fourier transformation, but this is not the case. We

introduce a set $\{|\varphi_{\alpha}^{(\mathbf{r})}\rangle\}$ of orbitals such that $n_{\mathbf{r}}$ is diagonal in this basis. The eigenvectors $|\varphi_{\alpha}^{(0)}\rangle$ of $n_{\mathbf{r}=0}$ and those $|\varphi_{\alpha}^{(\mathbf{r})}\rangle$ of other sites \mathbf{r} are connected by translation and also by a unitary transformation, or change of basis set. Picking $\mathbf{r} = \hat{e}_l$, $l = x$ means $\hat{e}_l = (1, 0)$ or transfer by one step towards the right and $l = y$ means $\hat{e}_l = (0, 1)$ or transfer by one step upwards. The unitary transformation reads:

$$|\varphi_{\alpha}^{(\hat{e}_l)}\rangle = \sum_{\beta=1}^{2N_{\Lambda}-2} |\varphi_{\beta}^{(0)}\rangle \langle \varphi_{\beta}^{(0)} | \varphi_{\alpha}^{(\hat{e}_l)} \rangle \equiv \sum_{\beta=1}^{2N_{\Lambda}-2} |\varphi_{\beta}^{(0)}\rangle T_{l\beta\alpha}. \quad (20)$$

The transfer matrix T_l knows all the translational and point symmetry of the system, and will turn out to be very special.

For large N_{Λ} , to find $\{|\varphi_{\alpha}^{(\mathbf{r})}\rangle\}$ it is convenient to separate the \mathbf{k} 's of \mathcal{S}_{hf} in irreducible representations of the space Group $\mathbf{G} = C_{4v} \otimes \mathbf{T}$. Choosing an arbitrary $\mathbf{k} \in \mathcal{S}_{hf}$ with $k_x \geq k_y \geq 0$, the set of vectors $R_i \mathbf{k}$, where $R_i \in C_{4v}$, is a (translationally invariant) basis for an irrep of \mathbf{G} . The high symmetry vectors $(0, \pi)$ and $(\pi, 0)$ always transform among themselves and are the basis of the only two-dimensional irrep of \mathbf{G} , which exists for any N_{Λ} . If $N_{\Lambda}/2$ is even, one also finds the high symmetry wavevectors $\mathbf{k} = (\pm\pi/2, \pm\pi/2)$ which mix among themselves and yield a four-dimensional irrep. In general, the vectors $R_i \mathbf{k}$ are all different, so all the other irreps of \mathbf{G} have dimension 8, the number of operations of the point Group C_{4v} .

Next, we show how to build our *local* basis set and derive $W = 0$ states for each kind of irreps of \mathbf{G} . For illustration, we shall first consider the case $N_{\Lambda} = 4$; then \mathcal{S}_{hf} contains the bases of two irreps of \mathbf{G} , of dimensions 2 and 4. The one with basis $\mathbf{k}_A = (\pi, 0)$, $\mathbf{k}_B = (0, \pi)$ breaks into $A_1 \oplus B_1$ in C_{4v} .

The eigenstates of $(n_{\mathbf{r}=0})_{ij} = \langle \mathbf{k}_i | n_{\mathbf{r}=0} | \mathbf{k}_j \rangle$, with $i, j = A, B$, are $|\psi''_{A_1}\rangle = \frac{1}{\sqrt{2}}(|\mathbf{k}_A\rangle + |\mathbf{k}_B\rangle)$ with $\lambda_1 = 1/8$ and $|\psi''_{B_1}\rangle = \frac{1}{\sqrt{2}}(|\mathbf{k}_A\rangle - |\mathbf{k}_B\rangle)$ with $\lambda_2 = 0$. Since under translation by a lattice step T_l along the $l = x, y$ direction $|\mathbf{k}\rangle \rightarrow e^{ik_l} |\mathbf{k}\rangle$, using Eq. (20) one finds that $|\psi''_{A_1}\rangle \leftrightarrow (-1)^{\theta''_l} |\psi''_{B_1}\rangle$, with $\theta''_x = 1$, $\theta''_y = 0$; so $|\psi''_{A_1}\rangle$ has vanishing amplitude on a sublattice and $|\psi''_{B_1}\rangle$ on the other. The two-body state $|\psi''_{A_1}\rangle_{\sigma} |\psi''_{B_1}\rangle_{-\sigma}$ has occupation for spin σ but not for spin $-\sigma$ on the site $\mathbf{r} = 0$; under a lattice step translation it flips the spin and picks up a (-1) phase factor: $|\psi''_{A_1}\rangle_{\sigma} |\psi''_{B_1}\rangle_{-\sigma} \leftrightarrow |\psi''_{B_1}\rangle_{\sigma} |\psi''_{A_1}\rangle_{-\sigma}$; therefore it has double occupation nowhere and is a $W = 0$ state ($W = 0$ pair[52],[51]).

The 4-dimensional irrep with basis $\mathbf{k}_1 = (\pi/2, \pi/2)$, $\mathbf{k}_2 = (-\pi/2, \pi/2)$, $\mathbf{k}_3 = (\pi/2, -\pi/2)$, $\mathbf{k}_4 = (-\pi/2, -\pi/2)$ breaks into $A_1 \oplus B_2 \oplus E$ in C_{4v} ; letting $I = 1, 2, 3, 4$ for the irreps A_1 , B_2 , E_x , E_y respectively, we can write down all the eigenvectors of $(n_{\mathbf{r}=0})_{ij} = \langle \mathbf{k}_i | n_{\mathbf{r}=0} | \mathbf{k}_j \rangle$, with $i, j = 1, \dots, 4$, as $|\psi'_I\rangle = \sum_{i=1}^4 O'_{Ii} |\mathbf{k}_i\rangle$, where O' is a 4×4 orthogonal matrix. The state with non-vanishing eigenvalue is again the A_1 eigenstate. After a little bit of algebra we have shown[61] that under T_l the subspace of A_1 and B_2 symmetry is exchanged with the one of E_x and E_y symmetry. Thus we can build a 4-body eigenstate of W with vanishing eigenvalue: $|\psi'_{A_1} \psi'_{B_2}\rangle_{\sigma} |\psi'_{E_x} \psi'_{E_y}\rangle_{-\sigma}$. As before under a lattice step translation this state does not change its spatial distribution but $\sigma \rightarrow -\sigma$ without any phase factor: $|\psi'_{A_1} \psi'_{B_2}\rangle_{\sigma} |\psi'_{E_x} \psi'_{E_y}\rangle_{-\sigma} \leftrightarrow |\psi'_{E_x} \psi'_{E_y}\rangle_{\sigma} |\psi'_{A_1} \psi'_{B_2}\rangle_{-\sigma}$.

Now we use these results to diagonalize $n_{\mathbf{r}=0}$ on the whole set \mathcal{S}_{hf} (we could have done that directly by diagonalizing 6×6 matrices but we wanted to show the general method). The eigenstate of $n_{\mathbf{r}=0}$ with nonvanishing eigenvalue always belongs to A_1 . The matrix $n_{\mathbf{r}}$ has eigenvalues $3/8$ and (5 times) 0 , as predicted by Eq. (19). For $\mathbf{r} = 0$ the eigenvector of occupation $3/8$ is $|\varphi_1^{(0)}\rangle = \frac{1}{\sqrt{3}}|\psi''_{A_1}\rangle + \sqrt{\frac{2}{3}}|\psi'_{A_1}\rangle$. The other A_1 eigenstate of $n_{\mathbf{r}=0}$ has 0 eigenvalue and reads: $|\varphi_2^{(0)}\rangle = \sqrt{\frac{2}{3}}|\psi''_{A_1}\rangle - \frac{1}{\sqrt{3}}|\psi'_{A_1}\rangle$. The other eigenvectors, whose symmetry differs from A_1 , are $|\varphi_3^{(0)}\rangle = |\psi'_{B_2}\rangle$, $|\varphi_4^{(0)}\rangle = |\psi''_{B_1}\rangle$, $|\varphi_5^{(0)}\rangle = |\psi'_{E_x}\rangle$ and $|\varphi_6^{(0)}\rangle = |\psi'_{E_y}\rangle$. One finds[61] that the transfer matrices T_l of Eq. (20) such that $|\varphi_I^{(\hat{e}_l)}\rangle \equiv \sum_J |\varphi_J^{(0)}\rangle T_{lJI}$, are *antiblock diagonal*. Thus, the local basis at any site \mathbf{r} splits into the subsets $\mathcal{S}_a = \{|\varphi_1^{(0)}\rangle, |\varphi_2^{(0)}\rangle, |\varphi_3^{(0)}\rangle\}$, and $\mathcal{S}_b = \{|\varphi_4^{(0)}\rangle, |\varphi_5^{(0)}\rangle, |\varphi_6^{(0)}\rangle\}$; a shift by a lattice step sends members of \mathcal{S}_a into linear combinations of the members of \mathcal{S}_b , and conversely.

Consider the 6-body eigenstate of K

$$|\Phi_{AF}\rangle_\sigma = |\varphi_1^{(0)}\varphi_2^{(0)}\varphi_3^{(0)}\rangle_\sigma |\varphi_4^{(0)}\varphi_5^{(0)}\varphi_6^{(0)}\rangle_{-\sigma}.$$

In this state there is partial occupation of site $\mathbf{r} = 0$ with spin σ , but no double occupation. It turns out that a shift by a lattice step produces the transformation

$$|\Phi_{AF}\rangle_\sigma \longleftrightarrow -|\Phi_{AF}\rangle_{-\sigma}$$

that is, a lattice step is equivalent to a spin flip, a feature that we have already met in Section 4.1 (*antiferromagnetic property*). Since the spin-flipped state is also free of double occupation, $|\Phi_{AF}\rangle_\sigma$ is a $W = 0$ eigenstate. A ground state which is a single determinant is a quite unusual property for an interacting model like this.

Note that $|\varphi_1^{(0)}\varphi_2^{(0)}\rangle$ is equivalent to $|\psi''_{A_1}\psi'_{A_1}\rangle$, because this is just a unitary transformation of the A_1 wave functions; so $|\Phi_{AF}\rangle_\sigma$ can also be written in terms of the old local orbitals (without any mix of the local states of different irreps of \mathbf{G}):

$$|\Phi_{AF}\rangle_\sigma = |\psi''_{A_1}\psi'_{A_1}\psi'_{B_2}\rangle_\sigma |\psi''_{B_1}\psi'_{E_x}\psi'_{E_y}\rangle_{-\sigma}. \quad (21)$$

This form of the ground state lends itself to be generalised to arbitrary even N_Λ , see Refs.[60],[61].

A few further remarks about $|\Phi_{AF}\rangle_\sigma$ are in order. (1) Introducing the projection operator P_S on the spin S subspace, one finds that $P_S|\Phi_{AF}\rangle_\sigma \equiv |\Phi_{AF}^S\rangle_\sigma \neq 0$, $\forall S = 0, \dots, N_\Lambda - 1$. Then, ${}_\sigma\langle\Phi_{AF}|W|\Phi_{AF}\rangle_\sigma = \sum_{S=1}^{N_\Lambda-1} {}_\sigma\langle\Phi_{AF}^S|W|\Phi_{AF}^S\rangle_\sigma = 0$, and this implies that there is at least one ground state of W in \mathcal{H} for each S . The actual ground state of H at weak coupling is the singlet $|\Phi_{AF}^0\rangle_\sigma$. (2) The *existence* of this singlet $W = 0$ ground state is a direct consequence of the Lieb theorem[25]. Indeed the maximum spin state $|\Phi_{AF}^{N_\Lambda-1}\rangle_\sigma$ is trivially in the kernel of W ; since the ground state must be a singlet it should be an eigenvector of W with vanishing eigenvalue. (3) The above results and Lieb's theorem imply that higher order effects split the ground state multiplet of H and the singlet is lowest. (4) The Lieb theorem makes no assumptions concerning the lattice structure; adding the ingredient of the \mathbf{G} symmetry we are able to explicitly display the wave function at weak coupling.

Energy	Irrep of \mathcal{G}	Degeneracy
4	\tilde{B}_2	1
2	Λ_4	4
0	Ω_4	6
-2	Λ_1	4
-4	A_1	1

Table 4. One-body spectrum of the 4×4 Hubbard model for $t = -1$. We have used the notation introduced in Ref.[65] in labelling the irreducible representations.

Using the explicit form of $P_{S=0}$ one finds that $P_{S=0}|\Phi_{AF}\rangle_\sigma = -P_{S=0}|\Phi_{AF}\rangle_{-\sigma}$. This identity allows us to study how the singlet component transforms under translations, reflections and rotations. In particular the *antiferromagnetic property* tells us that the total momentum is $K_{tot} = (0, 0)$. To make contact with Ref.[62] we have also determined how $|\Phi_{AF}^0\rangle$ transforms under the C_{4v} operations with respect to the center of an arbitrary plaquette. It turns out[61] that it is even under reflections and transforms as an s wave if $N_\Lambda/2$ is even and as a d wave if $N_\Lambda/2$ is odd.

In the next Section we use these results, together with the non-perturbative canonical transformation, to study the doped 4×4 lattice at half filling. Since the non-interacting ground state at half filling is now well known and unambiguously defined, the expansion (12) can be performed in a unique way.

4.3. Pairing in the Doped Hubbard Antiferromagnet

The one-body spectrum of the 4×4 Hubbard model has 5 equally spaced levels, see Table 4. The space Group \mathbf{G} [containing the translations and the 8 C_{4v} operations] can not explain the degeneracy 6, since in the 4×4 lattice the largest dimension of the irreps is 4. As observed by previous authors[63],[64], the 4×4 lattice can be mapped into the $2 \times 2 \times 2 \times 2$ hypercube since each pair of next to nearest neighbor sites has two nearest neighbor sites in common. This implies that H is invariant under a new and largest symmetry Group; let us call it \mathcal{G} .

Due to the importance of the symmetry in our configuration interaction mechanism, we have explicitly calculated the character table of \mathcal{G} taking into account an extra non-isometric symmetry operation[65]. \mathcal{G} has 384 elements, 20 classes and hence 20 irreps whose dimensionality fully justifies the degeneracies of Table 4.

As observed in Section 4.1 the canonical transformation applies when two holes are added to a non-degenerate vacuum. To study the system at and close to half filling, we have to use the results of Section 4.2. In the following we will solve the problem of two electrons added to the half filled system.

4.3.1. $W = 0$ Pairs In order to study the $W = 0$ pairing in the doped 4×4 antiferromagnet, we consider $W = 0$ pairs in the six-fold degenerate one-body level

[belonging to Ω_4]. Exploiting the $W = 0$ theorem, we have found[65] $W = 0$ pairs with symmetry Γ_1 , Γ_2 , Σ_2 , Ω_1 and triplet pairs with symmetry Σ_3 , Ω_2 , Ω_3 . Here, we are using the notation of Ref.[65]; the irreps Ω have dimension 6, the Σ 's have dimension 3 and Γ 's have dimension 2.

Exact diagonalization results[32] show that for $U/t < 3$ and $16 - 2 = 14$ holes the ground state is sixfold degenerate. Below, we use the canonical transformation and prove that the ground state corresponds to an Ω_1 $W = 0$ *electron* pair over the half-filled system. For $U/t > 3$ and the same number of holes a level crossing takes place: the ground state is threefold degenerate and contains a state with momentum $(0, 0)$ and a doublet with momentum $(\pi, 0)$ and $(0, \pi)$. Again, the computed ground state can be assigned to a Σ_2 *electron* pair over the half filled system[65].

4.3.2. Pairing mechanism We consider the ground state of the 4×4 Hubbard model with 14 holes; aside from the 10 holes in the inner A_1 and Λ_1 shells (see Table 4), the outer Ω_4 shell contains 4 holes. We intend to show how pairing between two *electrons* added to the antiferromagnetic 16-holes ground state (half filling) comes out. We use the antiferromagnetic ground state $|\Phi_{AF}^{S=0}\rangle$ as the non-interacting ground state of the configuration interaction expansion (12). With respect to this *electron vacuum*, the m states are now $W = 0$ pairs of *electrons* added to $|\Phi_{AF}^{S=0}\rangle$. In the 4×4 lattice the one-body energy levels are widely separated and the dominant interaction is between electrons in the same shell. Therefore, we consider as m states only the $W = 0$ electron pairs in the shell \mathcal{S}_{hf} , *i.e.*, those belonging to the irreps Ω_1 and Σ_2 , and we neglect the high-lying unoccupied orbitals. Explicit calculations[65] show that the effective interaction is attractive for both Ω_1 and Σ_2 $W = 0$ electron pairs and that the corresponding binding energy is $\Delta_{\Omega_1} = -61.9$ meV and $\Delta_{\Sigma_2} = -60.7$ meV for $U = -t = 1$ eV. Therefore, the weak coupling ground state can be interpreted as an Ω_1 $W = 0$ electron pair over the antiferromagnetic ground state. This result agrees with exact diagonalization data[32].

5. Carbon Nanotubes and Triangular Cobalt Oxides

5.1. Nanotubes

There is experimental evidence that the critical temperature T_c in alkali-graphite intercalation compounds C_xM (where M is a given alkali metal) grows as x decreases[66]. Under high-pressure, high metal concentration samples such as C_6K , C_3K , C_4Na , C_3Na , C_2Na , C_2Li have been synthesized; for C_2Na the value of T_c is 5 K while for C_2Li , $T_c=1.9$ K. Recently, Potassium[67] and Lithium[68] have been intercalated also in ropes of single- and multi-wall carbon nanotubes (the highest metal concentration was obtained with Lithium in C_2Li), and a net charge transfer between the alkali-metals and the carbon atoms has been predicted[69]. The alkali-metals cause little structural deformation, but increase the filling of the original bands. Nanotubes close to half filling are deemed to be Luttinger liquids down to milli-Kelvin temperatures[70],[71].

Here[72], we use the Hubbard Hamiltonian H on the wrapped honeycomb lattice to represent the valence bands of single-wall carbon nanotubes (SWNT) and we apply our symmetry-driven configuration interaction pairing mechanism based on the existence of $W = 0$ pairs. We shall focus on armchair (N, N) SWNT and show that the pair binding energy grows as the number of electrons per C atom increases. Furthermore, a stronger binding in nanotubes than in graphite sheets is predicted which suggests a higher critical temperature in the former. This is also supported by the measurements of a $T_c \approx 15$ K in the 4 Angstrom SWNT by Tang *et al.*[3].

Any armchair SWNT has a bonding (-) and an antibonding (+) band, and the Fermi line has C_{2v} symmetry (C_{6v} is the symmetry group of the graphite sheet). Since these systems are usually doped with *electrons*, we take the Fermi level ε_F to lie in the antibonding band. We use the $W = 0$ theorem for electrons with opposite quasimomentum and we find $W = 0$ pairs belonging to the pseudoscalar irrep A_2 of C_{2v} . Let (a, b) denote the basis of the Bravais lattice and $u(\mathbf{k}, \zeta)$ the periodic part of the Bloch function of quasi-momentum \mathbf{k} , with $\zeta = a, b$. The singlet pair wavefunction reads[72]

$$\begin{aligned} \psi_{\zeta_1, \zeta_2}^{[A_2]}(\mathbf{k}, \mathbf{R}_1, \mathbf{R}_2) &= \frac{1}{\sqrt{2}} \sin(k_x(X_1 - X_2)) \times \\ &\times \left[u^*(\mathbf{k}, \zeta_1) u^*(-\mathbf{k}, \zeta_2) e^{ik_y(Y_1 - Y_2)} - u^*(\mathbf{k}, \zeta_2) u^*(-\mathbf{k}, \zeta_1) e^{-ik_y(Y_1 - Y_2)} \right], \end{aligned}$$

with $\mathbf{R}_i = (X_i, Y_i)$ the origin of the cell where the particle i lies. We can verify by direct inspection that the $W = 0$ pair wavefunction $\psi^{[A_2]}$ vanishes for $X_1 = X_2$, that is if the particles lie on the same annulus of the armchair tube.

The effective interaction W_{eff} between the particles of a $W = 0$ pair can be obtained analytically by the canonical transformation approach described in Section 3.2. We let $\varepsilon(\mathbf{k})$ be the one-body energy excitation with momentum \mathbf{k} in the antibonding band and we call $\mathcal{D}/4$ a quarter of the empty part of the FBZ. The effective Schrödinger equation for the pair reads

$$[2\varepsilon(\mathbf{k}) + W_F + F(\mathbf{k}, E)] a_{\mathbf{k}} + \sum_{\mathbf{k}' \in \mathcal{D}/4} W_{\text{eff}}(\mathbf{k}, \mathbf{k}', E) a_{\mathbf{k}'} = E a_{\mathbf{k}}, \quad (22)$$

where W_F is the first-order self-energy shift (which we found to be independent of \mathbf{k}) and $F(\mathbf{k}, E)$ is the forward scattering term (which does not contains any direct interaction between the particles of the pair). Eq. (22) requires a self-consistent calculation of E (since W_{eff} and F are E -dependent). We show below that $E = 2\varepsilon_F + W_F + F_{\text{min}}(\mathbf{k}_F) + \Delta$, with a positive binding energy $-\Delta$ of the $W = 0$ pair; here $F_{\text{min}}(\mathbf{k}_F)$ is the minimum value of $F(\mathbf{k}, E)$ among the \mathbf{k}_F -wavevectors on the Fermi line.

First, we got a direct verification that pairing actually occurs in the $(1, 1)$ nanotube of length $L = 2$ (in units of the lattice spacing) and periodic boundary conditions. As for the CuO_4 , we compute the quantity $\tilde{\Delta}(4) = E(4) + E(2) - 2E(3)$ and we compare it with Δ (obtained from the canonical transformation). $\tilde{\Delta}(4)$ has been computed in a large range of U/t values, and its trend is shown in Fig. 8(a). In Fig. 8(b) it is reported the comparison between $\tilde{\Delta}(4)$ and Δ . We observe that the analytical value $|\Delta|$ is ~ 2

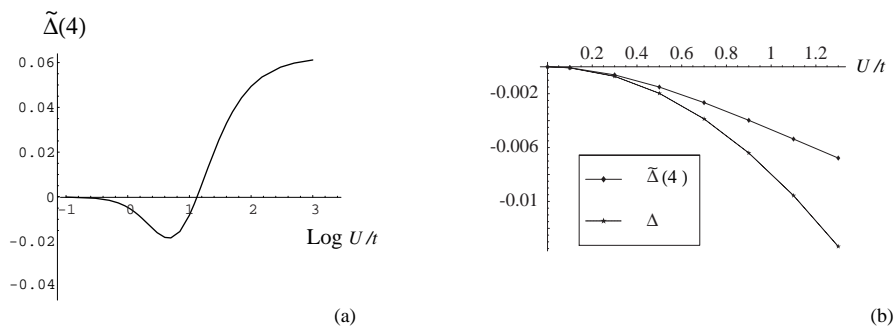


Figure 8. (a) Trend of $\tilde{\Delta}(4)$ in units of t versus $\text{Log } U/t$ in the range $-1 \div 3$ for the (1,1) nanotube. (b) Comparison between Δ and $\tilde{\Delta}(4)$.

times greater than $|\tilde{\Delta}(4)|$ for $U/t \simeq 1$, as for the CuO_4 cluster. However, the analytical approach predicts the right trend of the binding energy and it is very reliable in the weak coupling regime.

Next, we consider supercells of $2N \times L = N_C$ cells, where L is the length of the (N, N) nanotube in units of the lattice spacing. We solve the Cooper-like equation (22) in a virtually exact way for N up to 6 and L up to 25, using $U/t = 2.5$ (which is of the correct order of magnitude for graphite[73],[74]). The canonical transformation overestimates Δ in this range of U/t , but remains qualitatively correct. The calculations are performed with the Fermi energy ε_F varying between $0.8t$ and $1.1t$ (half filling corresponds to $\varepsilon_F = 0$). As in the (1,1) nanotube, the $W = 0$ pairs get bound once dressed by the electron-hole excitations. However, the binding energy $-\Delta$ decreases monotonically both with the radius and the length of the tube.

With supercell sizes $N_C > 300$ numerical calculations become hard and the AEI scheme is used in order to get reliable extrapolations. The AEI V_{eff} remains fairly stable around $\approx 1.5 \div 2t$ for $N > 2$ with increasing L . Furthermore, V_{eff} is largely independent of the Fermi energy. The weak dependence of V_{eff} on the length L allows for extrapolating the asymptotic value of the binding energy $\Delta_{\text{asympt}}(N) = \lim_{L \rightarrow \infty} \Delta(N, L)$, see also Section 3.4. The results are shown in Fig. 9(a) with $V_{\text{eff}} = 1.5t$. We found that Δ_{asympt} is strongly dependent on the filling at fixed N ; the sharp maximum at the *optimal doping* $\varepsilon_F \approx t$ (which corresponds to a number of electrons per graphite atom of 1.25) can be understood in terms of a corresponding peak in the density of states. In the *optimally doped* case $-\Delta_{\text{asympt}}(N)$ decreases monotonically as the radius of the tube increases, see Fig. 9(b). The decreasing of the binding energy with N is suggested by recent measurements on nanotubes with diameter of few Angstrom[3]. However, in the limit of large N , $\Delta_{\text{asympt}}(N)$ remains stable around $0.0028t$ and may be interpreted as the binding energy of the $W = 0$ pair in an *optimally doped* graphite sheet.

We emphasize that our pairing mechanism uses degenerate electronic states that exist in $2d$ (or quasi $2d$) and works away from half filling. A proper account for the transverse direction is crucial in order to have a non-Abelian symmetry group and hence $W = 0$ pairs. The $\psi^{[A_2]}$ pair wavefunction vanishes when the transverse component

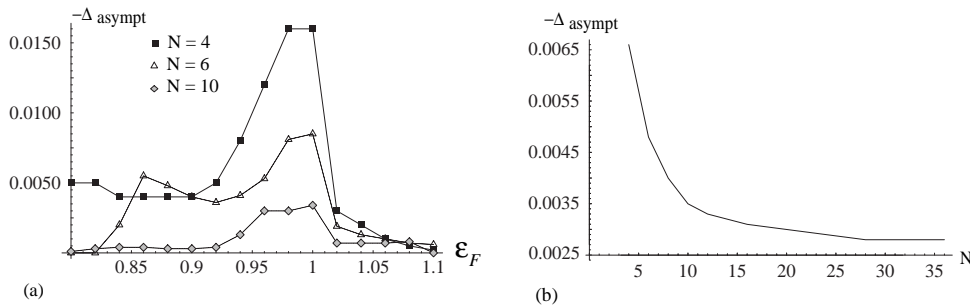


Figure 9. (a) Results of the canonical transformation approach with $U/t = 2.5$. $-\Delta_{\text{asympt}}$ as a function of the Fermi energy ϵ_F for $N = 4$ (black boxes), $N = 6$ (empty triangles) and $N = 10$ (grey diamonds). The Fermi energy varies in the range $0.8 \div 1.1$ t . (b) $-\Delta_{\text{asympt}}$ as a function of N for N in the range $6 \div 36$ with $\epsilon_F = t$ and Average Effective Interaction $V = 1.5$ t . In both figures $-\Delta_{\text{asympt}}$ is in units of t .

$k_y = 0$. This opens up the interesting possibility that in nanotubes two distinct superconducting order parameters appear in the phase diagram, if it turns out that close to half-filling there is another one which breaks down the Luttinger liquid.

5.2. Triangular Lattice in $W = 0$ Theory

We have also considered a symmetric triangular Hubbard lattice, which may be relevant to the newly discovered[5] Na_xCoO_2 superconductors which are now exciting considerable interest[75],[76]. The 7 atom centered hexagonal cluster with open boundary conditions yields no pairing for any filling. When opposite sites of this cluster are identified, one obtains a 4-site cluster which is the smallest one with periodic boundary conditions. With a hopping integral $t = -1$ we find that $\tilde{\Delta}(4)$ is negative and shows a similar trend versus U as in the CuO_4 case; the pairing energy exceeds $0.1t$ for $U \sim 4|t|$.

6. Superconducting Flux Quantization

Bulk superconductors quantize the flux through a hole in half-integer multiples of the fluxon ϕ_0 , because the quasiparticles that screen the vector potential carry charge $2e$. In finite systems the signature of superconductivity is a ground state energy minimum at $\phi = 0$ that is separated by a barrier from a second minimum at $\phi = \phi_0/2$. With increasing the size of the system, the energy (or free energy, at finite temperature) barrier separating the two minima becomes macroscopically large, and bulk superconductors can swallow up only half integer numbers of flux quanta. As emphasized by Canright and Girvin[77], the flux dependence of the ground state energy is definitely one of the most compelling ways of testing for superconductivity, and the existence of the two minima separated by a barrier is a strong indication of superconducting flux quantization.

6.1. General Group Theory Aspects of Cu-O Systems

In the present problem, with a repulsive Hubbard model, the mechanism of attraction is driven by the C_{4v} symmetry, and cannot operate in an unsymmetric geometry. The flux must be inserted in such a way that the system is not distorted. In the following we consider Cu-O systems with C_{4v} symmetry with respect to a central Copper ion, and insert the magnetic flux in such a way that only 4 central triangular plaquettes feel a magnetic field (see Figs. 10 and 11) and the rest of the plane only experiences a vector potential.

Consider the pattern of Fig. 10. Here, the Cu sites are marked by black dots and the Oxygen sites by empty dots; the X's stand for tubes carrying flux ϕ each, symmetrically disposed around the central Cu. According with the Peierls prescription we include the

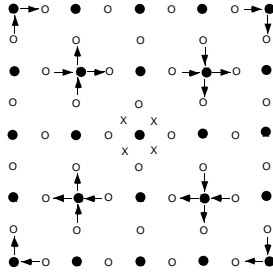


Figure 10. Pattern of the vector potential A due to 4 flux tubes (crosses) carrying flux ϕ . black dots stand for Cu atoms and empty dots stand for O sites. The line integral of A along each bond parallel to the arrow is $\frac{\phi}{2}$.

magnetic effects in the Hubbard model by setting

$$t_{jj'} \rightarrow t_{jj'} e^{\frac{2\pi i}{\phi_0} \int_j^{j'} \mathbf{A} \cdot d\mathbf{r}},$$

where $\phi_0 = 2\pi/e$ is the flux quantum and j and j' are the position of the two lattice sites connected by $t_{jj'}$. Varying ϕ by an integer multiple of ϕ_0 corresponds to a gauge transformation leaving all the physical properties unchanged. The arrows help to visualise a convenient choice of the gauge at general ϕ . Namely, running along an oriented bond in the sense of the arrow, $\int_{\rightarrow} \mathbf{A} \cdot d\mathbf{r} = \frac{\phi}{2}$; along the other Cu-O bonds, not marked in the figure, $\int \mathbf{A} \cdot d\mathbf{r} = 0$. One sees that in this way the flux through any closed path corresponds to the number of tubes surrounded by the path. The reflection operations of C_{4v} are equivalent to $\phi \rightarrow -\phi$, reverse the directions of the arrows and for a generic ϕ the symmetry Group reduces to Z_4 . However, at $\phi = \frac{\phi_0}{2}$ the reversal of the magnetic field in the tubes corresponds to a jump by ϕ_0 , and this is equivalent to a gauge transformation: this implies that the symmetry Group gets larger, the new symmetry operations being reflections supplemented by a gauge transformation. Indeed, the hopping parameter $t_{jj'}$ becomes $it_{jj'}$ along the arrows, while it remains equal to $t_{jj'}$ along the unmarked bonds of Fig. 10(a). Any reflection operation simply changes the signs of all the hoppings along the marked bonds. Now consider the unitary

transformation S which changes the signs of all the Cu orbitals along both diagonal, except the central Cu. Since S also has the effect of reversing all the arrows, $\sigma \times S$ is a symmetry, for all reflections σ in C_{4v} . Moreover, since the product of two reflections is a rotation, the Group \tilde{C}_{4v} including the rotations and the reflections multiplied by S is isomorphic to C_{4v} . The $W = 0$ pairs appropriate for half a flux quantum must involve two holes belonging to the degenerate irrep of \tilde{C}_{4v} . In this way, at $\phi = \frac{\phi_0}{2}$ the full symmetry is restored, allowing again for pairing and negative Δ . If pairing also occurs at $\phi = \frac{\phi_0}{2}$, the superconducting flux quantization arises from a level crossing between the ground state associated with the paired state at $\phi = 0$ and the ground state associated with the paired state at $\phi = \frac{\phi_0}{2}$.

6.2. Application to the CuO_4 Case and Numerical Results

As an illustrative application of the previous symmetry argument, let us investigate one more time the CuO_4 cluster. We expect that this system is a very good candidate to exhibit superconducting flux quantization, since it hosts two $W = 0$ pairs of different symmetries. As discussed above, this condition is necessary for the development of a level crossing.

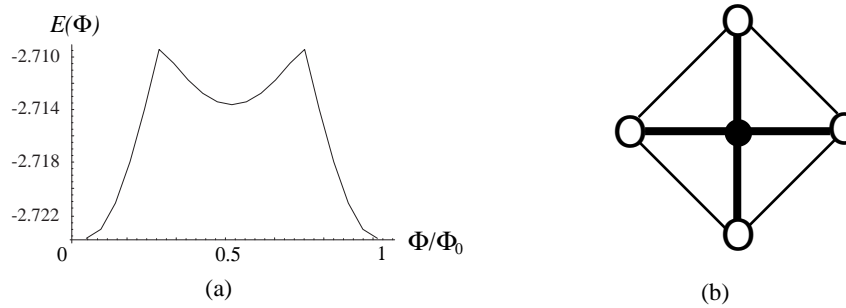


Figure 11. (a) Ground state energy of the CuO_4 with four holes as a function of ϕ/ϕ_0 . For ϕ/ϕ_0 between 0 and 1/4 and between 3/4 and 1 the ground state has B_2 symmetry; for ϕ/ϕ_0 between 1/4 and 3/4 it belongs to A_1 . Here $t = 1\text{eV}$, $t_{pp} = -0.01\text{eV}$, $U = 5\text{eV}$; $E(4, \phi)$ is in eV. (b) Topology of the CuO_4 cluster in presence of ϕ ; the crosses stand for flux tubes.

In agreement with the previous prescription, we have to insert 4 flux tubes around the central Copper [see Fig. 11(b)] in order to introduce a closed path around the center, where screening currents can respond. Every O-O bond collects the Peierls phase $\frac{2\pi i}{\phi_0} \int \mathbf{A} \cdot d\mathbf{r} = 2\pi i \frac{\phi}{\phi_0}$; by symmetry, t is unaffected by the flux. Thus, the Hamiltonian reads as in Eq. (5) with

$$t_{pp} \rightarrow t_{pp} e^{2\pi i \frac{\phi}{\phi_0}}.$$

We observe that a flux of the order of a fluxon in a macroscopic system would be a small perturbation; in the small cluster, however, the perturbation is small only if the hopping integral $|t_{pp}|$ is taken small compared to t . Numerically, the computations were performed with $t_{pp} = -0.01\text{ eV}$. By exact diagonalization, we have found that the ground

state energy $E(\phi)$ of the CuO_4 with 4 holes, as a function of ϕ , has clearly separated minima at zero and half a flux quantum [see Fig.11(a)]. Furthermore, $\tilde{\Delta}(4)$ is negative both at $\phi = 0$ and $\phi = \phi_0/2$: $\tilde{\Delta}(\phi = 0) = -43\text{meV}$ and $\tilde{\Delta}(\phi = \phi_0/2) = -32\text{meV}$.

The physical interpretation of Fig. 11(a) is the following. When the magnetic flux is inserted into the system, the $W = 0$ pair of B_2 symmetry creates a diamagnetic supercurrent that screens the external field. Such a current flows through the O-O bonds and form closed loops. As ϕ grows the energy of the system also increases, signaling that the $W = 0$ pair is spending its binding energy to screen the field. At a quarter fluxon a level crossing occurs, producing a second minimum at $\phi = \phi_0/2$. Here the Hamiltonian is real again and the A_1 pair is energetically favoured. As the flux increases further, the A_1 pair produce a new diamagnetic supercurrent until the initial situation is restored at $\phi = \phi_0$. The pairing state at zero flux and half fluxon are orthogonal. There is a clear analogy with the BCS theory; in that case, the Cooper wavefunction has s symmetry and the total magnetic quantum number of the pair vanishes in the absence of flux, but not at half a flux quantum.

It is worth to note that if the Hubbard repulsion U is set to zero, the second minimum at half a fluxon disappears and a trivial paramagnetic behaviour is observed. This is a further evidence that the superconducting behaviour of the system is induced by repulsion.

6.3. Rings of Symmetric Clusters

We have also studied[78],[79],[80] bound pair hopping and Superconducting Flux Quantization (SFQ) in systems with CuO_4 units as nodes of a graph Λ . For such systems the Hamiltonian is $H_{\text{tot}} = H_0 + H_\tau$ with

$$H_0 = \sum_{\alpha \in \Lambda} [t \sum_{i\sigma} (d_{\alpha\sigma}^\dagger p_{\alpha,i\sigma} + p_{\alpha,i\sigma}^\dagger d_{\alpha\sigma}) + U(n_{\alpha\uparrow}^{(d)} n_{\alpha\downarrow}^{(d)} + \sum_i n_{\alpha,i\uparrow}^{(p)} n_{\alpha,i\downarrow}^{(p)})],$$

while H_τ is an intercell hopping Hamiltonian. Here, $p_{\alpha,i\sigma}^\dagger$ is the creation operator for a hole onto the Oxygen $i = 1, \dots, 4$ of the α -th cell and so on. The point symmetry group of H_0 includes $S_4^{|\Lambda|}$, with $|\Lambda|$ the number of nodes. We shall consider an intercell hopping which preserves the S_4 subgroup of $S_4^{|\Lambda|}$ in order to have $W = 0$ pair solutions.

6.3.1. O-O Hopping and SFQ Consider a hopping term that allows a hole in the i -th Oxygen site of the α -th unit to move towards the i -th Oxygen site of the β -th unit with hopping integral $\tau_{\alpha\beta} \equiv |\tau_{\alpha\beta}| e^{i\theta_{\alpha\beta}}$:

$$H_\tau = \sum_{\alpha, \beta \in \Lambda} \sum_{i\sigma} \tau_{\alpha\beta} p_{\alpha,i\sigma}^\dagger p_{\beta,i\sigma}.$$

For $N = 2|\Lambda|$ and $\tau_{\alpha\beta} \equiv 0$, the unique ground state consists of 2 holes in each CuO_4 unit. The intercell hopping produced by small $|\tau_{\alpha\beta}| \ll |\tilde{\Delta}(4)|$ allows for studying the propagation of p pairs added to a background $2|\Lambda|$ holes. When U/t is such that $\tilde{\Delta}(4) < 0$, each pair prefers to lie on a single CuO_4 and for $N = 2|\Lambda| + 2p$ the unperturbed

ground state is $2^p \times \binom{|\Lambda|}{p}$ times degenerate (since each CuO_4 can host two degenerate $W = 0$ pairs). In the low-energy singlet sector, the problem is solved analytically to second order in H_τ and mapped into an effective Hamiltonian for p hard-core bosons with a complex effective hopping integral \mathcal{J} that we have calculated analitically and studied as a function of the ratio U/t . For ring-shaped systems, the effective model is equivalent to the Heisenberg-Ising spin chain governed by the Hamiltonian

$$H_{\text{HI}} = \sum_{\alpha=1}^{|\Lambda|} \mathcal{J} [2\eta \sigma_\alpha^z \sigma_{\alpha+1}^z + e^{\frac{4i\pi}{|\Lambda|} \frac{\phi}{\phi_0}} \sigma_{\alpha+1}^+ \sigma_\alpha^- + e^{-\frac{4i\pi}{|\Lambda|} \frac{\phi}{\phi_0}} \sigma_\alpha^+ \sigma_{\alpha+1}^-] \quad (23)$$

where the σ 's are Pauli matrices, spin up represents an empty site and spin down represents a pair. η is the so called anisotropy parameter and in our case $\eta = -1$. For $\eta = 1$, we have the isotropic Heisenberg interaction. By performing a Jordan-Wigner transformation, the Hamiltonian in Eq. (23) can also be mapped into a model of spinless fermions on the ring. In the absence of a threading magnetic field ($\phi = 0$) the problem was originally studied by Bloch[81] and then exactly solved by Hulthen[82] [in the case $\eta = -1$] and Orbach[83] [in the case $\eta \leq -1$] using the Bethe's hypothesis[84]. A systematic analysis in the whole range of parameters was given by Yang and Yang in a self-contained series of papers[85]. Here we just recall that the model has a gapless phase if $|\eta| \leq 1$, corresponding to the conducting state, while an insulating phase sets in for $\eta < -1$. As in the 1d Hubbard model, the “magnetic perturbation” ($\phi \neq 0$) does not spoil the integrability and the Heisenberg-Ising Hamiltonian remains exactly solvable by the Bethe-ansatz method. Let us write an eigenfunction of H_{HI} as

$$a(\alpha_1, \dots, \alpha_p) = \sum_P A_P e^{i \sum_j k_{Pj} \alpha_j}$$

where P is a permutation of the integers $1, \dots, p$ and A_P are $p!$ coefficients. Shastry and Sutherland[86] have shown that the variables k_j are given by

$$|\Lambda| k_j = 2\pi I_j + 4\pi \frac{\phi}{\phi_0} - \sum_{l \neq j} \theta(k_j, k_l) \quad (24)$$

with a phase shift

$$\theta(k, q) = 2 \tan^{-1} \left[\frac{\eta \sin[(k - q)/2]}{\cos[(k + q)/2] - \eta \cos[(k - q)/2]} \right].$$

From Eqs. (23)-(24) we readily see that the ground state energy of the low-energy effective Hamiltonian H_{HI} is periodic with period $\phi_0/2$, independent of the number of added pairs. Thus we conclude that the purely repulsive CuO_4 -Hubbard ring threaded by a magnetic field quantizes the flux in a superconducting fashion if the number of particles is $2|\Lambda| + 2p$ with $0 \leq p \leq |\Lambda|$.

For rings of 2 and 3 CuO_4 -sites, we also confirmed the analytic results by exact diagonalization; for the three- CuO_4 ring we observed the SFQ with total number of holes $2|\Lambda| + 2 = 8$. The switching on of the hopping τ between the Oxygen sites breaks the symmetry group $C_{3v} \otimes S_4^3$ into $C_{3v} \otimes S_4$ for real τ ; in a magnetic field (complex

τ), this further breaks into $C_3 \otimes S_4$. Real τ lifts the degeneracy between the $k = 0$ subspace and the subspaces $k = 1$ and $k = 2$ of C_3 (as usual k is related to the crystal momentum $p \equiv 2\pi\hbar k/3$ in this case), but cannot split $k = 1$ and 2 because they belong to the degenerate irrep of C_{3v} ; complex τ resolves this degeneracy.

The three-CuO₄ ring is the smallest ring where we can insert a magnetic flux ϕ by $\tau = |\tau|e^{i\theta}$, $\theta = \frac{2\pi}{3}(\phi/\phi_0)$. The energies of the three ground-state multiplet components are reported in Fig. 12(a) for $|\tau| \ll |\tilde{\Delta}(4)|$ and $U = 5t$. At $\phi = 0$ the ground state

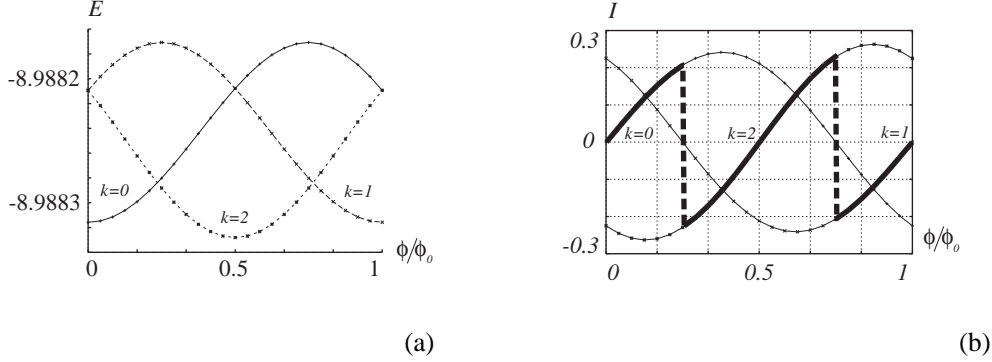


Figure 12. (a) Numerical results for the low energy states of the three-CuO₄ ring, as a function of the concatenated magnetic flux. The energy is in units of t . (b) Total current for the three-CuO₄ ring, as a function of the magnetic flux. The current is in units of $e|\tau|/h$. In both figures, $U = 5t$, $[\tilde{\Delta}(4) \approx -0.04258t]$ $|\tau| = 0.001t$.

belongs to the $k = 0$ subspace, while the first excited levels have $k = 1$ and 2 . Their spatial degeneracy is fully lifted: the $k = 1$ level increases while the $k = 2$ level decreases up to $\phi = \phi_0/2$. As ϕ increases, the ground state energy grows quadratically in ϕ (diamagnetic behaviour). Near $\phi = \phi_0/4$ we find a level crossing between $k = 0$ and $k = 2$, while at $\phi = \phi_0/2$, $k = 0$ becomes degenerate with $k = 1$ and the ground state energy is in a new minimum belonging to the $k = 2$ subspace: a sort of “restoring” of the $\phi = 0$ situation is taking place as in the BCS theory[87]. Indeed, at $\phi = \phi_0/2$ the symmetry group is $\tilde{C}_{3v} \otimes S_4$ where \tilde{C}_{3v} is isomorphous to C_{3v} (reflections σ are replaced by σg , where g is a suitable gauge transformation).

Fulfilling the conditions $\tilde{\Delta}(4) < 0$ and $|\tau| \ll |\tilde{\Delta}(4)|$, we have varied U and $|\tau|$ and found analogous trends for the ground state energy. Increasing $|\tau|$ with fixed $\tilde{\Delta}(4)$ lowers the central minimum and depresses the two maxima. On the other hand, if $|\tilde{\Delta}(4)|$ decreases at fixed $|\tau|$ the central minimum and the side peaks are affected in a similar way. This is reasonable since the perturbative parameter is $|\tau|/|\tilde{\Delta}(4)|$.

The current operator $\hat{I} = c\frac{\partial H_0}{\partial \phi}$ yields[88] a gauge invariant average I and in Fig. 12(b) we display I as a function of ϕ in the three ground state sectors $k = 1, 2$ and 3 . The current is proportional to the flux derivative of the ground-state energy [see Fig. 12(a)] according to the Hellmann-Feynman theorem and clearly shows a superconducting behaviour.

The ground state energy in each k sector for the non-interacting ($U = 0$) Cu₃O₁₂ ring shows no pairing in CuO₄ and indeed the ground state energy is linear in the field at

small fields (normal Zeeman effect). The lowest state is $k = 2$ throughout. The absence of SFQ is a further evidence of the repulsion-driven pairing mechanism discussed above. Thus, the dressed $W = 0$ pair screens the vector potential as a particle with an effective charge $e^* = 2e$ does. At both minima of $E(\phi)$ we have computed for the Cu_3O_{12} ring $\tilde{\Delta}(8) \approx -10^{-2}t$.

6.3.2. Cu-Cu Hopping: infinite effective mass The three- CuO_4 ring with $2|\Lambda| + 2 = 8$ holes contains a $W = 0$ pair which in the case $\tilde{\Delta}(4) < 0$ gets bound; an intercell hopping τ_{Cu} is now assumed between Cu sites only. This is perfectly able to carry a one-body current when the full system is threaded by the flux, and it does in the absence of interactions. However the bound pairs have an interesting behaviour. $|\tau_{\text{Cu}}| \ll |\tilde{\Delta}(4)|$ produces very much smaller effects on the energy than τ does, but anyhow the system behaves as a paramagnet and there is no flux-induced splitting of the three k levels. This happens because the $W = 0$ pair is strictly localized by the *local* symmetry. Indeed the S_4 label of each CuO_4 unit is a good quantum number. No SFQ is observed because the screening of the magnetic field by the bound pair is forbidden. The superconducting pair behaves as if it had a very large effective mass.

7. $W = 0$ Pairing and Electron-Phonon Interactions

The role of electron-phonon (EP) interactions in determining the superconducting correlations in the Cu-O planes of cuprates is a very controversial issue. Possibly, the pairing mechanism has a predominantly electronic origin, but many high- T_C compounds exhibit a quite noticeable doping-dependent isotope effect, suggesting that EP interactions could be important and should be included in the theory. In particular there is experimental evidence that the half breathing Cu-O bond stretching mode at $k = (\pi, 0), (0, \pi)$ is significantly coupled with the doped holes in the superconducting regime and its contribution may be relevant for the $d_{x^2-y^2}$ pairing[89].

Here we further investigate this issue by addressing the question if the $W = 0$ pairing available in the Hubbard model survives when the lattice degrees of freedom are switched on. When lattice effects are introduced in this scenario, several questions arise. In the conventional mechanism, phonons overscreen the electron repulsion; what happens if electronic screening already leads to pairing? It is not obvious that the phonons will reinforce the attraction while preserving the symmetry. More generally, some vibrations could be pairing and others pair-breaking. To address these problems we use an extension of the Hubbard model in which bond stretchings dictate the couplings to the normal modes of the C_{4v} -symmetric configuration, generating a long-range (Fröhlich) EP interaction.

We start from the Hubbard model with on-site interaction U and expand the hopping integrals $t_{i,j}(\mathbf{r}_i, \mathbf{r}_j)$ in powers of the displacements ρ_i around a C_{4v} -symmetric

equilibrium configuration

$$t_{i,j}(\mathbf{r}_i, \mathbf{r}_j) \simeq t_{i,j}^0(\mathbf{r}_i, \mathbf{r}_j) + \sum_{\alpha} \left[\frac{\partial t_{ij}(\mathbf{r}_i, \mathbf{r}_j)}{\partial r_i^{\alpha}} \right]_0 \rho_i^{\alpha} + \sum_{\alpha} \left[\frac{\partial t_{ij}(\mathbf{r}_i, \mathbf{r}_j)}{\partial r_j^{\alpha}} \right]_0 \rho_j^{\alpha},$$

where $\alpha = x, y$. Below, we write down the ρ_i^{α} in terms of the normal modes $q_{\eta\nu}$: $\rho_i^{\alpha} = \sum_{\eta\nu} S_{\eta\nu}^{\alpha}(i) q_{\eta\nu}$, where η is the label of an irreducible representation (*irrep*) of the symmetry group of the undistorted system and ν is a phonon branch.

Thus, treating the Cu atoms as fixed, for simplicity, one can justify an electron-lattice Hamiltonian:

$$H_{el-latt} = H_0 + V_{\text{tot}}.$$

Here $H_0 = H_0^n + H_0^e$ accounts for the kinetic part of the electron-phonon system and it is given by

$$H_0 = \sum_{\eta} \hbar \omega_{\eta,\nu} b_{\eta,\nu}^{\dagger} b_{\eta,\nu} + \sum_{i,j,\sigma} t_{i,j}^0(\mathbf{r}_i, \mathbf{r}_j) c_{i\sigma}^{\dagger} c_{j\sigma};$$

the ω 's are normal mode frequencies. The interacting part $V_{\text{tot}} = V + W$ contains the Hubbard repulsion W and the electron-phonon interaction V . The latter can be written in terms of the parameters $\xi_{\eta,\nu} = \lambda_{\eta\nu} \sqrt{\frac{\hbar}{2M\omega_{\eta,\nu}}}$, where the λ 's are numbers of order unity that modulate the EP coupling strength, while M is the Oxygen mass. Then,

$$V = \sum_{\eta,\nu} \xi_{\eta,\nu} (b_{\eta,\nu}^{\dagger} + b_{\eta,\nu}) H_{\eta,\nu},$$

and the $H_{\eta,\nu}$ operators are given by

$$H_{\eta,\nu} = \sum_{i,j} \sum_{\alpha,\sigma} \left\{ S_{\eta\nu}^{\alpha}(i) \left[\frac{\partial t_{ij}(\mathbf{r}_i, \mathbf{r}_j)}{\partial r_i^{\alpha}} \right]_0 + S_{\eta\nu}^{\alpha}(j) \left[\frac{\partial t_{ij}(\mathbf{r}_i, \mathbf{r}_j)}{\partial r_j^{\alpha}} \right]_0 \right\} (c_{i,\sigma}^{\dagger} c_{j,\sigma} + h.c.).$$

This is physically more detailed than the Hubbard-Holstein model, where electrons are coupled to a local Einstein phonon and the superconducting phase has been investigated in detail[90],[91]. Indeed, in the present context the Hubbard-Holstein model is not fully satisfactory because it restricts to on-site EP couplings, which would be impaired by a strong Hubbard repulsion. On the other hand the use of a Fröhlich-like phonons was suggested[92],[93],[94] for modeling the Cu-O planes in the strong EP coupling regime: a long-range EP coupling removes the problem of polaron self-trapping, otherwise present in the case of the Holstein interaction, where an unphysically large polaron (and bipolaron) mass occurs.

By generalizing to $H_{el-latt}$ the canonical transformation proposed for the electronic part $H = H_0^e + W$, one can derive[95],[96] an effective interaction between the particles in the pair. We obtained a new Cooper-like equation $H_{\text{pair}}|\varphi\rangle = E|\varphi\rangle$ with an effective two-body Hamiltonian, acting upon the dressed $W = 0$ pair $|\varphi\rangle$. As in Section 3 the pairing criterion involves the properly renormalized Fermi energy $E_F^{(R)}$: if the lowest energy eigenvalue E is such that $E = E_F^{(R)} + \Delta$ with negative Δ , the dressed $W = 0$ pair gets bound in the many-body interacting problem and the system undergoes a Cooper

instability. We observed that this extended approach is very accurate at weak coupling and is qualitatively predictive also in the intermediate coupling regime.

As an illustrative application we focussed again on CuO_4 . This cluster represents a good test of the interplay between electronic and phononic pairing mechanisms since we can compare exact diagonalization results with the analytic approximations of the canonical transformation. CuO_4 allows only the coupling to phonons at the centre or at the edge of the Brillouin Zone; however, phonons near the edge are precisely the most relevant ones[89]. We recall (see Section 2.2) that the pure Hubbard CuO_4 cluster with O-O hopping $t_{pp} = 0$ yields $\tilde{\Delta}(4) < 0$, and a degenerate $W = 0$ bound pair with A_1 and B_2 components. A standard Jahn-Teller calculation in which the degenerate ground state wave functions interact with the vibrations predicts distortions that already at moderate EP coupling destroy the pairing[96]. We also explored the scenario beyond this approximation. The analytical solution of the Cooper-like equation shows that the electronic pairing is enhanced by the phonon contribution. In particular the binding energy of the pair in the B_2 symmetry channel increases more rapidly than in the A_1 channel.

In order to go beyond the weak-coupling regime we have exactly diagonalized the Hamiltonian in a truncated Hilbert space. We obtained several indications. First, the catastrophic distortions predicted by the Jahn-Teller approximation are not borne out by more complete approaches involving a broader spectrum of electronic states. Pairing prevails also at strong coupling in part of the parameter space, in the symmetry channels where $W = 0$ pairs occur. The correct trend is predicted by the canonical transformation approach, which also explains the pairing or pair-breaking character of the individual normal modes. In particular it is found that the half-breathing modes give a synergic contribution to the purely electronic pairing; since they are believed to be mainly involved in optimally doped cuprates, our findings suggest a joint mechanism, with the Hubbard model that captures a crucial part of the physics.

8. Conclusions and Outlook

We have presented the following evidence that the $W = 0$ pairs are the quasi-particles that, once dressed, play the rôle of Cooper pairs: 1) as two-body states they do not feel the large on-site repulsion, that would come in first-order perturbation in any theory of pairing with any other kind of pairs. 2) The indirect interaction with the background particles gives attraction, and bound states with physically appealing binding energies. 3) The same results are also borne out by exact diagonalization in finite clusters, if and only if they have the correct symmetry and filling to give raise to $W = 0$ pairs in partially filled shells. 4) Both in clusters and in the plane, the superconducting flux quantization results from the symmetry properties of $W = 0$ pairs.

The setup of our theory of the effective interaction W_{eff} between two holes (or electrons) is quite general; although we developed it in detail for Hubbard Models, it is well suited to be extended in order to include other ingredients, like phonons. In

principle we can obtain W_{eff} by our canonical transformation, including systematically any kind of virtual intermediate states. The closed-form analytic expression of W_{eff} we obtained includes 4-body virtual states. This describes repeated exchange of an electron-hole pair to all orders. One can envisage the pairing mechanism by spin-flip exchange diagrams that are enhanced by the C_{4v} symmetry. The argument does not depend in any way on perturbation theory, and the equations retain their form, with renormalized parameters, at all orders. We find that in the three-band Hubbard Model, 1A_2 pairs are more tightly bound close to half filling, but 1B_2 pairs are favored when the filling increases. Here, like in the BCS theory, the superconducting flux quantization relies on the existence of bound pairs of different symmetries. We recall, however, that these symmetry labels are not absolute, but depend on the choice of a gauge convention. We get attraction and pairing at all fillings we have considered (above half filling), but the binding energy of the 1A_2 pairs drops by orders of magnitude as the filling increases. The three-band Hubbard Model might be too idealized to allow a detailed quantitative comparison with experiments; however some qualitative answers are very clear.

Using the Lieb's theorem[25] and a symmetry analysis based on the $W = 0$ theorem, one can fix the way the interactions remove the high degeneracy of the Hubbard Model at half filling. This can be used to study pairing in the doped system by the above canonical transformation. Exact numerical data on the 4×4 square lattice are available[32], and this allows to test the $W = 0$ pairing mechanism within the one-band Hubbard Model, improving over previous weak coupling analyses[48][49]. For a full application of the $W=0$ theorem, we had to include nontrivial symmetries which are no isometries; this enabled us to classify the $W = 0$ channels and calculate the binding energies analytically. Once the analysis is so complete, the criteria for pairing are unambiguous. Moreover the success of the weak coupling approach has been noted by other authors[97], and the reason is fully clarified by the $W = 0$ theory.

Despite some evident and important differences that we pointed out above, our mechanism can be thought of broadly speaking as a lattice realization of the pioneering one proposed long ago[12] by Kohn and Luttinger. The repulsion is avoided by the $W = 0$ configuration mixing without using parallel spins and high angular momenta. The basic source of attraction, however, is essentially the same, since in second-order, in the singlet channel, the spin-flip diagram is the only one that survives. We found pairing in the singlet channel in a variety of models including carbon nanotubes[72]. This real-space approach is suitable for realizing thought experiments, like those involving the SFQ (Section 6).

On the other hand, the above results also prove that important ingredients are still missing and must be included. The 4×4 model shows evidence of bound pairs of non-vanishing momentum, in degenerate representations. This opens up the possibility of charge inhomogeneities and Jahn-Teller distortions. However modeling vibration effects in a CuO_4 cluster we find that the outcome depends on which phonon mode is most strongly coupled. The bound pairs can be flexible enough to prevent distortions and actually gain binding energy in the presence of A and B phonons, whilst E vibrations

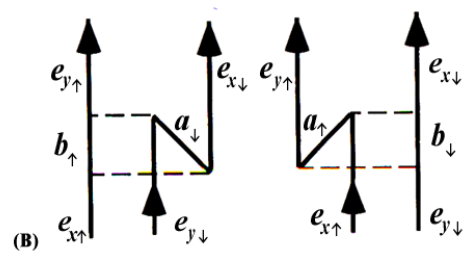
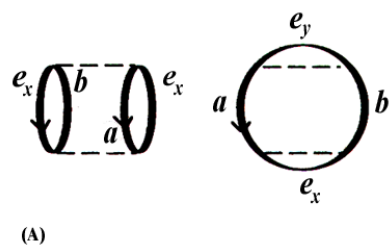
are definitely pair breaking.

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A_1 symmetry

T_1 symmetry $(S_4) = B_1 + E (C_4)_{4v}$

A_1 symmetry